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(Basic Research Programs)

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ENERGY DEVELOPMENT AND APPLICATIONS

OF THE

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SCIENCE AND TECHNOLOGY
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November 1984

DOE/ER-0146/1
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Office of Basic Energy Sciences
1984 Summary Report

A summary of the
organization, mission, and
activities of the Office of
Basic Energy Sciences

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Washington, D.C. 20545

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The Office of Basic Energy Sciences is one of several program offices in the Department of Energy's Office of Energy Research and plays an important role in the support of basic research in the United States today. The program is strongly oriented toward developing the information and understanding required for the long-term technological capability of the nation. This program is organized along the disciplinary lines of research science to effectively interact with the scientific community. The program summaries that describe the BES subprograms are also organized by scientific disciplines, but the basic research conducted under the auspices of several of our divisions often has a common underlying energy theme. A survey of research activities relevant to improving our insight into problems and solutions of long-term nuclear waste isolation, for instance, will span several disciplines. Conversely, a given project can impact more than one energy technology; this illustrates the merits of basic research.

This report is a summary document on the Basic Energy Sciences program, its overall scope, the kinds of activities carried out, and the unique facilities that have become a key part of our ability to conduct forefront research.

Donald K. Stevens

Donald K. Stevens
Deputy Associate Director for Basic Energy Services

Introduction

Over the years, a tradition of leadership in science and technology has evolved in the United States that has led other nations to emulate us. Today it is our basic research activity, carried out mainly in universities and government laboratories that underpins continuing U. S. leadership in science, provides for the training of future scientists, and contributes to our social and economic well-being. Our national goals—better health and quality of life for all our people, economic growth, energy self-sufficiency, national security, reduction in the arms race, etc.—involve technological advances that depend on basic research. Knowledge and discoveries resulting from research provide the foundation for new ideas and concepts to stimulate technology development and economic growth.

This past year, for example, saw the selection of a new material developed at DOE's Oak Ridge National Laboratory as one of the 100 best technology achievements in the United States for 1983. The material, nickel aluminide with minor alloying additions, is one of a class of lightweight structural alloys that are a direct outgrowth of continuing basic research to understand the relationship of the properties of materials to their structure and composition at the atomic level.

Nickel aluminide already is attracting industrial interest. Through alloying, it can be made ductile and easy to fabricate; it is made of lightweight and inexpensive materials; and it is six times stronger than stainless steels at high temperatures. This newly developed alloy overcomes a major problem that has prevented the wide use of intermetallic compounds like the aluminides for structural applications. The nickel aluminides are strong and resistant to corrosion and high temperatures but, until this development, were too brittle to be suited to structural applications. At room temperature, this new material's strength is comparable to commercial superalloys, and it actually becomes stronger at higher temperatures. This example illustrates how basic research contributes to continued technological innovation; the prospects for early commercialization of this new material for structural applications are promising.

Basic research is a painstaking activity requiring long-term commitments of resources and people with little promise of early success or return on investments. Thus the support of long-range basic research has emerged as the particular responsibility of the federal government as the only institution with the motivation, capability, and continuity to carry it through.

This report briefly describes the program of the Department of Energy's Office of Basic Energy Sciences, which is responsible for basic research in the scientific disciplines from which contributions to our long-term energy goals are likely to come. The Basic Energy Sciences subprograms and facilities are discussed, along with an abbreviated budget summary and an outline of plans for the future. Reports referenced are normally available from the National Technical Information Service, U. S. Department of Commerce, Springfield, VA 22161.

Overview

The Office of Basic Energy Sciences (BES), which reports to the Department of Energy's (DOE) Director of Energy Research, is the office responsible for long-range basic energy-related research and is charged with providing the fundamental scientific foundation on which the nation's future energy options depend. The organization of BES, which is primarily discipline oriented, is shown in Fig. 1. Research is sponsored in selected areas of the traditional scientific disciplines—the physical and biological sciences, geosciences, and engineering. The subprograms of BES support approximately 1200 individual research projects, each one selected on the basis of its scientific merit, its possible relevance to meeting the BES long-range research goals, and its contribution toward a balanced, responsive research program.

The knowledge that results from BES-sponsored research becomes a part of the body of information on which the applied technologies rest. Although research to broaden the technology base needed for identified energy options is extremely important, even more important is the need for basic research, unfettered by preconceived notions of what technologies will be important several decades from now, so that new, not yet identified options may emerge. Because of its diversified interests, with centralized management and common goals, BES can respond quickly and efficiently to DOE and national missions. The scientists and engineers of BES include professionals with years of experience in fostering and conducting creative basic research and managing major complex research facilities.

Any discussion of BES must consider that:

- BES is oriented toward DOE's energy mission.
- BES is a major participant in the physical and engineering sciences efforts of the nation.
- BES is a principal source of support of university research and of the national laboratories.
- BES is involved in the construction and operation of large and complex scientific facilities.

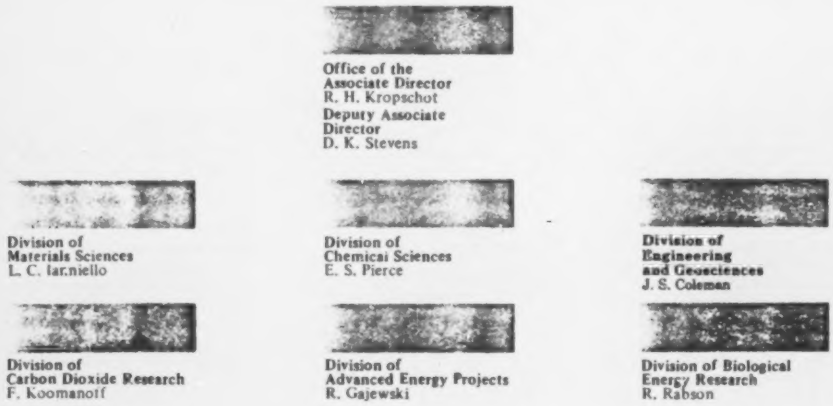
The energy supply and conservation missions of DOE are so vital to the nation's future that a comprehensive program of basic energy- related research is essential. It is the responsibility of BES to plan and administer DOE's program of basic research in the physical, biological, and engineering sciences exclusive of high-energy and nuclear physics and the medical and environmental sciences. The multipurpose national laboratories are national assets and play an essential role in U. S. science and technology, maintaining expert scientific and engineering staffs, building and operating complex scientific facilities, and undertaking large interdisciplinary projects. A large fraction of the BES budget goes to the national laboratories to support research, much of it dependent on complex facilities and services at the laboratories.

Basic Energy Sciences has a heavy involvement in scientific facilities (e.g., the National Synchrotron Light Source at Brookhaven National Laboratory, the Combustion Research Facility at Sandia-Livermore, the High Flux Isotope Reactor at Oak Ridge National Laboratory, and high-voltage and atomic resolution microscopes). Many areas of modern science require large and costly facilities; without them the necessary research could not be done. The large, expensive, unique facilities in the BES program are made available to the entire basic research scientific community to the extent that funds permit the additional shifts of operation.

Most of the scientists involved in BES research programs are at universities and national laboratories. University research receives support in several ways, e.g., "financial plan" funding, in which rather large sums of money are allocated to institutions to support identified projects but the institution is delegated authority to manage the overall program of research; special research contracts (and, in the future, grants) to support the research of individual scientists with graduate assistants, which is the largest form of university support; and support of two national laboratories that are co-located with universities—Lawrence Berkeley Laboratory at the University of California and Ames Laboratory at Iowa State University. In addition, free access by qualified scientists is provided to user facilities at national laboratories. More than one-third of BES funding supports university-based research. An important fringe benefit resulting from supporting research in universities is the research training of graduate students who continue in R&D after completion of their studies.

In addition to universities and national laboratories, BES maintains ties with industry. Representatives of appropriate industries serve on counseling committees for several of the BES subprograms; experts from industry participate in the review of research proposals and use the specialized facilities

Figure 1 Office of Basic Energy Sciences organizational chart.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Division of
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and Geosciences
J. S. Coleman
Division of
Carbon Dioxide Research
F. Koomanoff
Division of
Advanced Energy Projects
R. Gajewski
Division of Biological
Energy Research
R. Rabson

sponsored by BES; industrial scientists participate in program advisory committees at the national laboratories; and industry representatives are invited to attend the BES conferences and workshops. Through these and other mechanisms available to and used by the scientific community, the results of the BES program are available to industry and to the academic community.

The Basic Energy Sciences program also is a participant in the Congressionally mandated Small Business Innovation Research program, which was initiated in Fiscal Year 1983. A number of BES projects are being supported at highly specialized, research-oriented small business firms. The level of this effort was 0.6% of the BES research budget in Fiscal Year 1984—i.e., about $1,500,000—and will increase to 1% in Fiscal Year 1985 and 1.25% in Fiscal Year 1986.

The Office of Basic Energy Sciences evolved from the Division of Physical Research of the Atomic Energy Commission. The Office expanded its activities with the formation of the Energy Research and Development Administration in 1975 and again with the establishment of DOE in 1977. Each transition broadened the scope of its responsibilities for research in energy technologies, e.g., from nuclear to fossil, solar, and conservation. For over 35 years, BES has responded to the needs for basic research in areas of national priority.

Research in BES is conducted under seven subprograms: Materials Sciences; Chemical Sciences; Nuclear Sciences; Engineering and Geosciences; Advanced Energy Projects; Biological Energy Research; and Carbon Dioxide Research. At present, programmatic priorities call for emphasis in the areas of Biological Energy Research, Advanced Energy Projects, and Engineering and Geosciences. Other areas currently being emphasized include:

- High-temperature materials— corrosion, ceramics, and coatings
- Synthesis of novel materials
- Chemistry and physics of combustion processes
- Surface modification
- High-voltage and atomic resolution microscopy
- Condensed matter theory
- Amorphous materials
- Chemical structure and behavior of coal
- Structural ceramics
- Synchrotron radiation research
- Catalytic mechanisms and surface phenomena
- Neutron scattering research
- Photochemistry
- Nuclear data for fusion reactions
- Nondestructive evaluation

Each of the subprograms is described briefly in the following chapter. The major objective of BES—to provide the basic scientific knowledge and insight necessary to develop new and improved energy options—is pursued through several concurrent approaches, some already identified. They are to:

- Provide critical knowledge and data and develop trained scientific talent through support of highly competent researchers in DOE mission areas
- Provide for and support the operation of unique, specialized research facilities
- Maintain liaison with other DOE programs, federal agencies, and the scientific, academic, and industrial communities
- Seek the scientific and industrial communities' identification of needs and opportunities for research in areas likely to be relevant to future energy options
- Expand research into new areas identified as having potential importance to energy
- Promote application of the results of basic research

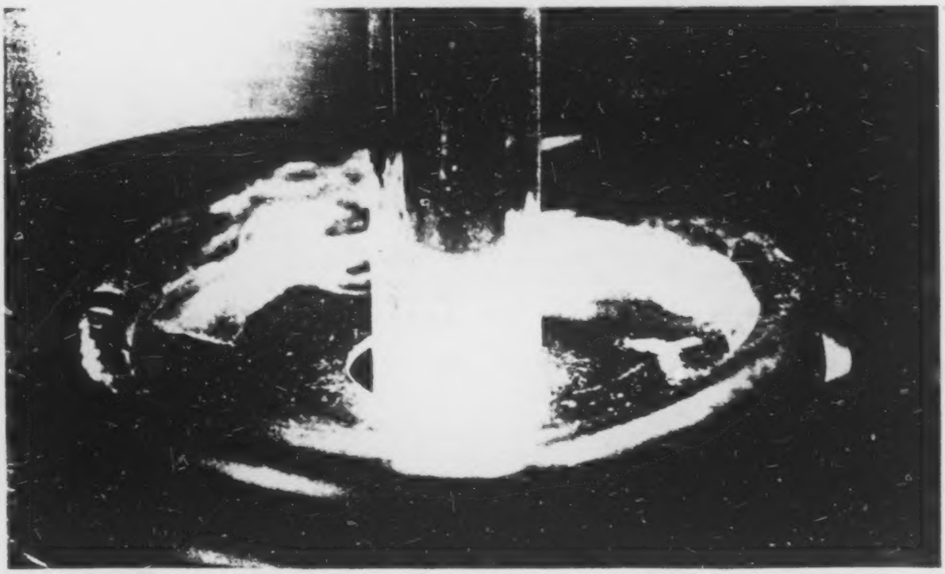
Interagency information exchanges, committee interactions, and workshops provide useful liaison between BES and other research groups. For example, DOE offices and laboratories and such federal agencies as the National Science Foundation, the Nuclear Regulatory Commission, and the U. S. Geological Survey have working groups and committees that routinely exchange information and coordinate program activities in such common research areas as nuclear data, chemistry, geophysics, hydrogen, materials, and combustion research. Coordinating committees discuss individual proposals and compare work being done by the various agencies to avoid overlap and duplication of effort. Outreach workshops and working groups bring together investigators in related areas to share information and discuss problem areas in their work. Finally, and most importantly, study results always are published in the open literature to make them available to the scientific community worldwide.

The Discovery of Glassy Metals and Their Future Potential

Questions often are raised about the role basic research plays in the mission of the Department of Energy or about its priority in relation to the near-term needs in the technologies being developed by the applied research of the Department. The development of a new class of materials called glassy, or amorphous, metals illustrates the long-term contribution of basic research. The genesis of glassy metals can be traced directly to basic research sponsored by the Materials Sciences subprogram 25 years ago. Glassy metals differ in structure and properties from metals as we usually think of them. Normally, metals have a crystalline structure, with atoms arranged in periodic arrays called lattices. In contrast, atoms in glassy metals do not form periodic arrays—their distribution is random. Originally devised a quarter of a century ago, the technique of producing amorphous metals requires cooling the molten metal about one hundred thousand times faster than had previously been possible. Extremely rapid cooling is the only way to prevent mobile atoms in the molten metal from rearranging themselves into crystal lattices. The amorphous metal produced with rapid cooling has been limited to very thin films because heat must be removed so quickly. Recently, more advanced techniques of materials science have been brought to bear on the problem of producing thicker samples, e.g., controlled diffusion of chemical elements into and out of the crystals, which causes them to become amorphous.

The current work grew out of methods of dealing with an early problem involving the empirical rules used by physical metallurgists to describe the formation of complete solid solutions in binary alloys. An exception to the rules was a copper-silver system that, on cooling, yielded two different solutions, both of very limited solubility, instead of the anticipated complete binary solution. It was thought that the molten mixture would be cooled rapidly enough to by-pass the reaction point and produce the expected solution. This took place in 1959.

The new, successful rapid cooling technique was applied to other binary systems, and new crystalline phases were produced. Within a few months, a non-crystalline gold-silicon metallic solution was found in an amorphous state similar to glass but having the electrical conductivity characteristic of a metal. By 1970, about 100 papers on metastable alloys and their properties had been published. It was concluded at that time that the inherent requirements of the heat-transfer process would always limit the thickness of



these "liquid-quenched metastable alloys" and any useful applications of them. Today, some 14 years later, new techniques of ion implantation and controlled diffusion have removed that limitation. Continuing research focuses on better understanding of this new approach, how to control it, and the nature of the resulting materials. Thus, advances in materials sciences have made feasible a current research goal of producing massive samples of amorphous metals rather than thin films.

The first uses for metallic glasses will be in magnetic applications. A unique feature of the amorphous structure is that it can be magnetized and demagnetized with lower losses of energy than can a crystalline structure. Energy losses that occur when the magnetic field is reversed are a problem in power transformers, where crystalline steels are now used throughout the United States. The losses in magnetic energy in these transformers are estimated to cost over six hundred million dollars per year; it has been estimated that most of this annual cost could be saved by substituting amorphous metals for the steels. There also are other magnetic applications—e.g., the recording and playback "heads" in tape recorders and the starting circuits in fluorescent lights. Thus, through technology transfer, the original research already is leading to significant commercial use of glassy metals in communication and lighting.

Subprograms

Materials Sciences

The goal of the Materials Sciences subprogram is to increase understanding of the phenomena and properties important to materials behavior; this understanding is essential to the development of future energy technologies. It is well-known that materials problems and limitations often restrict the performance of current energy systems and the development of future systems. Some needs to which Materials Sciences research ultimately contributes include:

- Developing new or substitute materials
- Tailoring materials to satisfy defined requirements
- Predicting materials problems and service life
- Improving the ability to successfully attack unforeseen materials problems in advanced energy systems
- Improving the theoretical and experimental capability to analyze the fundamental structure of materials

With support at an operating level of $125 million in FY 1984, the BES Materials Sciences subprogram provides about one-third of the total federal funding for basic materials research. Materials Sciences places emphasis on selected generic areas of fundamental importance and on areas where problems are known to exist or are anticipated. Some research is directed at a single energy technology (e.g., photovoltaic materials for solar energy conversion); some research has applicability to many technologies simultaneously (e.g., embrittlement of structural materials in the presence of hydrogen); and still other research has more fundamental implications underpinning all materials research (e.g., mechanisms of atomic transport in solids). The research is conducted in a variety of institutions—DOE laboratories, universities, and, to a lesser extent, industrial installations—and uses the talents of metallurgists, ceramists, solid-state physicists, and materials chemists.

In addition to maintaining an appropriate mix of long-term scientific, multitechnology, and single-energy-technology-related research, a balance must be retained among forefront, large, facility-related research and small individual projects. The Materials Sciences subprogram uses some major facilities in the pursuit of its research goals, including the National Synchrotron Light Source and the High Flux Beam Reactor (HFBR), both at Brookhaven National Laboratory; the Surface Modification and Characterization Collaborative Research Center and High Flux Isotope Reactor at Oak Ridge National Laboratory; the Intense Pulsed Neutron Source at Argonne National Laboratory; the high-voltage electron microscopes at Oak Ridge, Argonne, and Lawrence Berkeley Laboratories; and the Stanford Synchrotron Radiation Laboratory (SSRL) at Stanford University. The operation of these facilities required about 21% of the FY 1984 operating budget of the Materials Sciences subprogram, not including the research associated with them. Most of these facilities are unique, as is the research carried out at these sites. The facilities are also available to qualified users outside the DOE laboratory complex.

The agency's materials program is coordinated primarily through the DOE Energy Materials Coordinating Committee. The Materials Sciences subprogram is the basic materials program in DOE, which underpins the energy materials technologies. It represents about 20% of the total DOE materials research and development effort. The fact that there is four times as much effort in applied materials development is testimony to the crucial role materials play in the development of energy systems. Within the federal government, the subprogram is coordinated in part through the interagency Committee on Materials (COMAT). The workshops and reports of the subprogram's Council on Materials Science (a nongovernmental body with representatives from academia, industry, and agency laboratories) help to focus attention on critical issues. In 1983, panel meetings on coatings and surface modifications and on conducting organic materials were held. In 1984, the two meetings were on computer simulation and materials synthesis. The agency's applied materials research workers interact and exchange information through a number of mechanisms, including a formalized Research Assistant Task Force.

Current emphases and trends are toward greater use of the major facilities.

More detailed information on this subprogram can be obtained from Louis C. Ianniello, Director, Division of Materials Sciences, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545. A detailed summary of current projects is published annually. The most recent (September 1984) is entitled "Materials Sciences Program, Fiscal Year 1984" (DOE/ER-0143/2).

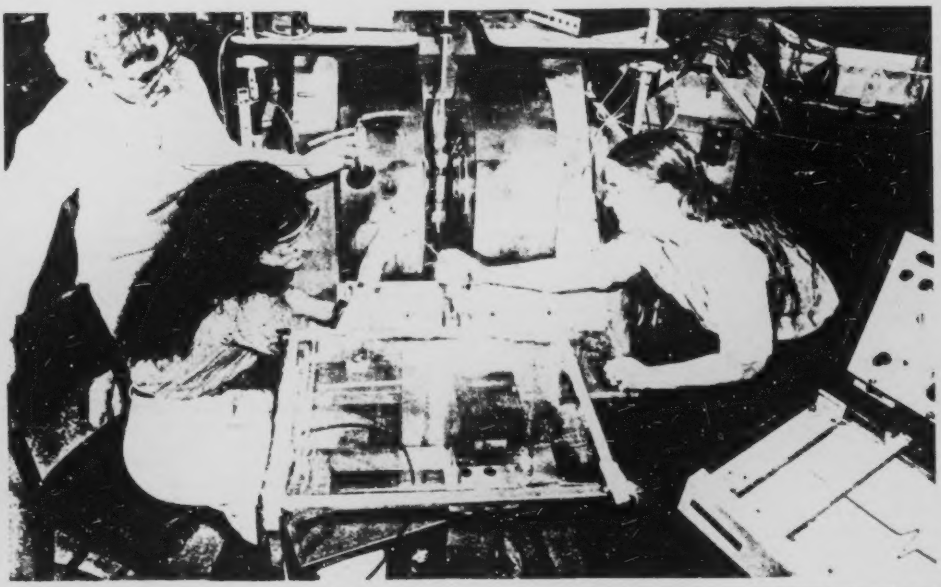
Chemical Sciences

The research activities supported by the Chemical Sciences subprogram range from energy-related phenomena involving liquids, gases, and plasmas to the chemical properties of solids, such as coal, chlorophyll, and catalysts, and the phenomena and behavior of submicroscopic particles, such as molecules, atoms, ions, and electrons.

The objective of Chemical Sciences is to expand the knowledge base in the chemical and related sciences in areas most likely to lead to new ideas and improved processes for developing and using domestic energy resources. At a budget level of $76 million, this subprogram is a major source of federal support for basic chemical research in the United States.

Phenomena and processes likely to be important to energy technologists are emphasized in the formulation of the program. Research in some areas, such as the chemical effects of catalysts, may lead to discoveries that can be quickly exploited by industrial process designers; whereas in others, such as water-splitting photochemistry to produce hydrogen, research may not be used for a number of years. Still other research areas, such as studies of radiation emitted by ions moving very fast through crystal foils, produce data for use in developing new energy technologies.

The Chemical Sciences subprogram includes research in the fields of photochemistry, coal chemistry, catalysis, atomic physics of highly charged ions, chemistry basic to nuclear waste separation, biomass conversion of liquid fuels by enzyme catalysis and other methods, energy-efficient separation of valuable metals from low-grade resources, efficient and clean combustion of various fuels, and detection and measurement of harmful by-products of energy processes. Equally important is the fundamental research into chemical and physical phenomena which has no immediately identifiable related technology. A typical example of such efforts is the study of laser-induced excited states of molecules. Disciplinary areas covered by Chemical Sciences work include physical, organic, and inorganic chemistry; chemical physics; radiation chemistry; thermodynamics; thermophysics; and analytical chemistry.



Much of the Chemical Sciences research centers on the special facilities at DOE's national laboratories—the Combustion Research Facility, National Synchrotron Light Source, electron linear accelerators, ion accelerators, superconducting nuclear magnetic resonance spectrometers, very advanced molecular beam machines, differential speed-of-light fiber optics, etc. In addition to their unique equipment, DOE laboratories provide enhanced opportunities for interactions between basic researchers and research and development teams in related energy technology areas. University laboratories carry out a large part of the remaining work, and a small part takes place in industrial laboratories. Laboratory scientists supported by Chemical Sciences also interact with industrial research workers, such as those in the automotive and petroleum industries.

Coordination with energy technology programs is emphasized. Laboratory-based interactions between the basic researchers in Chemical Sciences and the applied technology teams are assisted by headquarters-based coordination. Various conferences and committees—e.g., the Hydrogen Coordinating Committee, Solar Photochemistry Research Conferences, and Coal Chemistry and Catalysis Research Meetings—identify research needs and opportunities, compare results, and coordinate activities within DOE and with the rest of the scientific community. In addition, Chemical Sciences staff members serve as advisors for energy technology activities and visit and review activities at the DOE national laboratories.

Additional detailed information on the Chemical Sciences subprogram can be obtained from Elliot S. Pierce, Director, Division of Chemical Sciences, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545. A detailed summary of current projects is published annually. The most recent (September, 1984) is entitled *Summaries of FY 1984 Research in the Chemical Sciences* (DOE/ER-0144/2).

Nuclear Sciences

The objectives of the BES Nuclear Sciences subprogram are to:

- Measure, compile, and evaluate nuclear data for fission and fusion energy technologies
- Improve knowledge of the chemical and physical properties of the actinide elements
- Assure the availability for research of isotopically enriched samples of the elements
- Operate the Stanford Synchrotron Radiation Laboratory
- Conduct heavy ion fusion accelerator research

Nuclear Data

The fission and fusion energy technologies require nuclear data for optimization of reactor design, analysis of operations and safety of reactor systems, and management of spent fuel materials. The nuclear data activity provides a long-range base of data in support of these technologies. Nuclear data needs are documented in great detail and are regularly updated—for *fission* technology, through the work of the Cross Section Evaluation Working Group of the National Nuclear Data Center (NNDC), and for *fusion* technology, by means of a working group of the U. S. Nuclear Data Committee and DOE's Office of Fusion Energy.

The compilation and evaluation effort is concerned with establishing a data base for neutron-induced nuclear reactions and also with maintaining the Evaluated Nuclear Structure Data File (ENSDF), which encompasses all the information produced worldwide on the level structure and decay properties of nuclei.

The nuclear data compilation and evaluation effort is centered around the NNDC at Brookhaven National Laboratory, which coordinates a network of scientists performing compilation and evaluation for ENSDF and also coordinates U. S. work with the International Atomic Energy Agency. Data compilation and evaluation activities devoted to ENSDF and the publication of the Nuclear Data Sheets are monitored by an advisory panel of the National Academy of Sciences. Annually, NNDC processes about 700 requests for nuclear data from scientists and engineers in the energy technologies, biomedical scientists, and basic researchers.

The nuclear data measurement effort is centered around the Oak Ridge Electron Linear Accelerator for measurement of neutron cross sections over a wide range of energies. Several small university groups and the National Bureau of Standards collaborate in these activities.

Heavy Element Research

The nuclear energy and technology programs of DOE need specific information and data on the behavior of actinides in fuel processing streams, in nuclear waste hosts materials, and in the environment. Heavy element chemistry research helps meet their needs, as well as contributing to an understanding of the fundamental chemical and physical properties and behavior of matter. These broadly based studies of the actinide elements include behavior in aqueous and nonaqueous solutions, photochemistry, chemical reactivity, spectroscopy, and chemical physics.

Research groups at national laboratories and universities are supported to pursue heavy element (actinide) and radiochemical investigations. The study of actinide chemistry is largely limited to the national laboratories since high levels of radioactivity are involved, but some tracer work is done at universities. These laboratory facilities provide opportunities for visiting scientists from university and foreign labs to pursue collaborative research with the U. S. investigators. The heaviest elements are produced by irradiating curium-loaded targets in the High Flux Isotope Reactor (HFIR) and chemically processing the targets in the Transuranium Processing Plant (TRU) to extract and purify the actinide samples. These samples are allocated to investigators engaged in DOE research programs.

Isotopes Separations

Nuclear Sciences also supports the electromagnetic separation of stable isotopes for a Research Materials Collection of samples that are loaned out for nondestructive research in DOE energy technology programs. In addition to its research and information-gathering activities, Nuclear Sciences is responsible for distributing the stable isotopes and the rare, heavy radioactive isotopes it produces for use in research, medicine, and industry. These efforts constitute the western world's only source of isotopic research samples in significant quantities, and these materials are sold or loaned to institutions throughout the world.

Stanford Synchrotron Radiation Laboratory

Basic Energy Sciences is responsible for operating the Stanford Synchrotron Radiation Laboratory (SSRL). The SSRL was expanded under the auspices of the National Science Foundation in partial response to a National Academy of Sciences report that pointed out the potential for research in the newly identified area of synchrotron radiation. The SSRL, which shares the Stanford Positron Electron Asymmetric Ring with the high-energy physics program, is an important research facility; at present it is heavily oversubscribed by the solid-state, chemical, and biomedical research communities for its high-intensity photons in the ultraviolet and X-ray regions of energy. This is one of two major BES facilities where research of this kind is made possible.

Heavy Ion Fusion Accelerator Research

Research on heavy ion accelerators for potential application to inertial fusion is a recent addition to the energy mission of Basic Energy Sciences. The Heavy Ion Fusion Accelerator Research (HIFAR) program, a spinoff from high-energy accelerator physics, is managed by the Office of High Energy and Nuclear Physics. The program goal over the next several years is to establish a data base in accelerator physics and technology that can allow the promise of the accelerator approach to be accurately assessed.

The experimental program concentrates on developing a multiple-beam-induction linear accelerator (linac) to provide the necessary high-current beam of heavy ions. This type of accelerator has intrinsic characteristics that make it attractive as an inertial fusion driver:

- It is conceptually simple, involving a minimum number of beam manipulations.
- Adequate pulse repetition rates (30 to 100 pps) and good efficiency (15 to 25%) are expected.
- Considerable experience exists with kilo-ampere electron beams in induction linacs.
- The most serious technical issues of the method can be demonstrated in a small- to medium-sized accelerator.

These characteristics and, in general, the promise of this method of fusion energy have been verified in a number of national reviews, studies, and technical workshops.

The most important recent accomplishment in the HIFAR program was the development of conceptual designs for an accelerator to demonstrate a substantial fraction of the physics and engineering principles of a full-scale inertial fusion driver. Preliminary designs indicate, for example, that a heavy ion accelerator at one-tenth to one-twentieth of the cost of a fusion plant accelerator will demonstrate key design parameters at one-third full scale. Tests at this scale would provide the Department of Energy with an ample data base on which to base decisions on the future of this fusion method.

The accelerator to accomplish these goals has been named the High Temperature Experiment (HTE) because all the various tests of accelerator performance and a test of the heavy ion beam target interactions can be combined in one measurement; e.g., the temperature of the dense plasma produced by focusing the accelerated beam into a small spot on a plane slab target. Concurrently, recent experimental programs have shown that the highly space-charge-dominated ion beams required for such accelerators are feasible. This result has broad applications not only to fusion drivers but also to all high-current particle accelerators and thus is a spinoff of the HIFAR program.

Most of the current research activities in the HIFAR program are conducted at the Lawrence Berkeley Laboratory and the Los Alamos National Laboratory. The program is coordinated with the Office of Inertial Fusion within the Department's Defense Programs.

Additional information on the nuclear data activities can be obtained from Enloe Ritter, Director, Division of Nuclear Physics, Office of High Energy and Nuclear Physics; on the HIFAR program from Terry F. Godlove, Program Manager, Office of High Energy and Nuclear Physics; and on the other aspects of the Nuclear Sciences subprogram from Elliot S. Pierce, Director, Division of Chemical Sciences, Office of Basic Energy Sciences, all at the Department of Energy, Washington, DC 20545.

Engineering and Geosciences

The Engineering and Geosciences subprogram supports research in mechanical, structural, and electrical engineering; geology; geochemistry; and geophysics. Priorities are established through extensive interaction between experts in technological communities in the fields of interest, building on the well-documented studies of the Energy Research Advisory Board, the agency's comprehensive review of its own technology activities, and studies by the National Academy of Sciences and others.

The objective of engineering research is to advance the engineering science needed for energy production facilities and for increased energy efficiency. At present, three research areas are receiving high priority:

- Mechanical sciences, including tribology (the basic nature of friction-reduction phenomena), heat transfer, and solid mechanics (continuum mechanics and engineering aspects of crack propagation)
- Systems sciences, including process control, instrumentation, and scale-up of process plants
- Engineering analysis, including nonlinear dynamics, thermophysical properties of fluids, and engineering combustion

One of the current projects in tribology provides a useful example of the type of research under way. An attempt is being made to establish a sound experimental basis for a new theory of viscoelastic composites to predict the internal rolling friction of a tire. Automobile efficiency is reduced as a result of the rolling friction of tires—typically 10% or more of the engine horsepower is lost here. Eventually it should be possible to predict the best tire design to maximize fuel mileage without reducing tire life, traction, or safety—the three traditional tire performance criteria.

Engineering research also includes work on instrumentation for measuring basic engineering quantities—temperature, pressure, flow rates, and phase—under extreme conditions of temperature or pressure and efforts to model complex systems to develop predictive capabilities for the scale-up of pilot process plants.

The objective of the Geosciences program is to develop a quantitative, predictive understanding of the energy-related aspects of geological, geophysical, and geochemical processes both in the earth and at the solar–terrestrial interface.

The Geosciences program is emphasizing (1) long-range research on the geological isolation of nuclear waste, (2) studies in organic geochemistry relating to fossil fuel recovery and the disposition of energy-related chemical waste, and (3) studies of the magmahydrothermal part of the interagency Continental Scientific Drilling Program.

The effort in nuclear waste isolation addresses unresolved problems with second- and third-generation repositories (e.g., quantitative assessment of local changes of stress, with subsequent development of new fracture systems, which provide pathways for the migration of nuclear wastes; interactions among waste container, rock, and fluids in the rock; and concentrations, diffusion rates, and element migration of nuclear wastes from a disposal site into its surroundings).

The organic geochemical processes of migration, physical changes, and maturation of fossil energy resources are also being studied. Such knowledge is essential if fossil fuels are to be effectively exploited and is required for dealing with the problems of organic wastes.

The Magma Energy Research project, having demonstrated the scientific feasibility of extracting energy from magma bodies, has been phased out, but the DOE portion of the national Continental Scientific Drilling Program (CSDP) will continue to be focused on magmahydrothermal systems. A cooperative interagency program, CSDP seeks to develop an understanding of the North American continent. The DOE part will aid in predicting deposits of energy and mineral resources, establishing a scientific base of information relevant to nuclear waste isolation, and assessing hazards associated with the siting of major energy-related facilities. So far, programs of shallow and intermediate depth drilling have been initiated, and a drill-hole data base for holes drilled for the federal government has been established.

Other research involves rock mechanics, geodynamics, advanced geophysical techniques, resource definition and use, and solar–terrestrial relations.

More information on this subprogram can be obtained from James S. Coleman, Director, Division of Engineering and Geosciences, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545.

There are two reports available which supply more detailed information on this subprogram:

Summaries of FY 1984 Engineering Research, DOE/ER-0158/2, December 1984.

Summaries of Physical Research in the Geosciences, DOE/ER-0145/2, September 1984.

Advanced Energy Projects

The objective of the Advanced Energy Projects (AEP) subprogram is to explore the feasibility of novel energy-related concepts evolving from basic research which are at an early stage of scientific definition and, therefore, would not be of interest to technology programs. To qualify for AEP support, such concepts, even though they involve a high degree of risk, must have the potential for an eventual high payoff. Advanced Energy Projects also sponsors exploratory research on concepts that do not fit easily into the existing DOE program structure. An area of major attention is the transfer of successful projects to technology programs; a number of such transfers have already been made.

A relatively new BES subprogram, Advanced Energy Projects supports individual projects for a limited time only, with the goal of supporting about 20 new projects each year. It differs from other subprograms in that it does not fund ongoing, evolutionary research. After a period of concentrated effort, typically about 3 years, the concept is expected to have proved itself, in which case the basic research phase is completed and the project can be transferred to a technology program. If a successful conclusion to the research is not foreseeable, the project is dropped. Projects are selected from unsolicited proposals received from researchers at universities, industrial laboratories (especially small R&D companies), and national laboratories. Currently, 36 projects are being supported; this allows a turnover rate of about 12 projects per year.

Advanced Energy Projects is an interdisciplinary program whose projects cover a broad technological spectrum, e.g., new approaches to controlled fusion, completely new methods of solar energy concentration and collection, ultrasonic coal grinding, new heat engines, the development of X-ray lasers, and new methods of accelerating charged particles.

A recent accomplishment of this subprogram is a finding that fusion reactions, when "catalyzed" by elementary particles called muons, occur at a much higher rate than had been predicted when this approach to controlled fusion was first suggested in the 1950s. This realization, following from AEP-supported experiments proposed by scientists from the Idaho National Engineering Laboratory, could lead to a new look at this intriguing option of effecting fusion reactions at essentially room temperatures.

Additional information about the current activities of this subprogram is available from Ryszard Gajewski, Director, Division of Advanced Energy Projects, Office of Basic Energy Sciences, ER-16, Department of Energy, Washington, DC 20545. An annual report, *FY 1984 Research Summaries* (DOE/ER-0150/2, October 1984), also provides more detailed information on this subprogram.

Biological Energy Research

The principal objective of Biological Energy Research is to provide basic information and conceptual understanding in microbiological and botanical sciences for DOE's efforts in renewable resource production of fuels and chemicals, microbiological transformation of organic materials for conservation, and biological systems for resource recovery. The research is aimed at gaining an understanding of the underlying mechanisms of green plant productivity, converting biomass and other organic materials into fuel and chemicals by novel and improved methods of fermentation, and developing biosystems capable of saving energy.

The Biological Energy Research subprogram focuses on understanding the limits of productivity in green plants, how plants adapt to suboptimal conditions of growth, such as those encountered in marginal lands and waters, and the mechanisms of microbial conversion of various biomass forms. In particular, the biochemical pathways and their genetic and biochemical regulation relating to degradation of abundant materials such as cellulose, hemicelluloses, and lignins and the conversion of these materials to fuels or chemicals are studied.

Microorganisms that grow in the absence of oxygen and are able to carry out fermentation with high efficiency are of special interest, as are thermophilic microorganisms, which have optimal growth and conversion rates at high temperatures. An integral part of the subprogram is the development of genetic information that may ultimately be used to produce new or improved microorganisms and plants to facilitate the production of fuels or petroleum-conserving chemicals or to yield biotechnologies capable of conserving energy.

This research into the physiology, biochemistry, and genetics of microorganisms and plants is carried out primarily at university laboratories.

Further information on this subprogram can be obtained from Robert Rabson, Director, Division of Biological Energy Research, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545. Also available is the *Annual Report and Summaries of FY 1984 Activities* (DOE/ER-0147/2, October 1984), which provides detailed descriptions of ongoing activities.

Carbon Dioxide Research

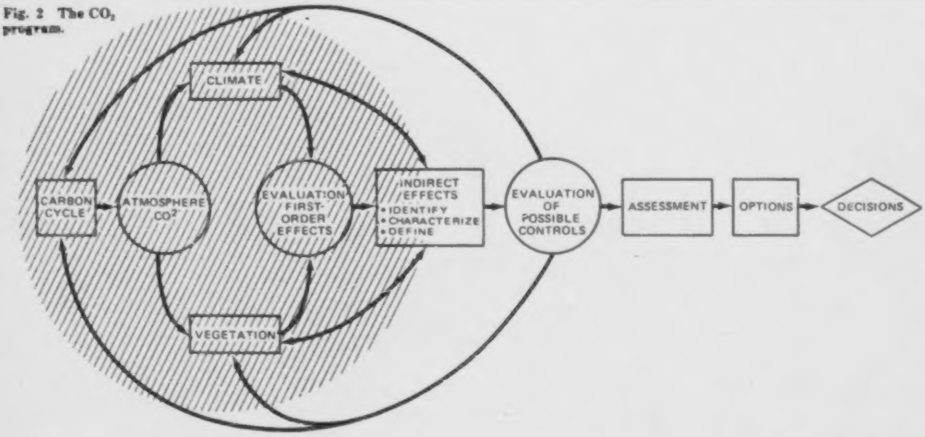
Detailed worldwide measurements indicate that the amount of carbon dioxide (CO_2) in the earth's atmosphere is gradually increasing. Scientific analysis suggests that such an increase could have substantial effects on climate and on agriculture and other human endeavors.

The goal of the Department of Energy's Carbon Dioxide Research Program is the identification of possible policy options for governmental action in response to these changes. The achievement of this goal requires a significant increase in our scientific knowledge of the atmosphere, the biosphere, the oceans, and the cryosphere—their interactions and the effects that increasing atmospheric CO_2 and other trace gases will have on them. To identify and specify choices that are valid, we must gather accurate scientific data and develop the necessary computer models through which we can:

- Project future atmospheric CO_2 concentrations
- Estimate CO_2-induced global and regional climate changes
- Estimate crop and ecosystem response to higher CO_2 concentrations
- Evaluate human health and welfare effects attributable to CO_2-induced climate and vegetation changes

With these data, it should be possible to consider innovative concepts and strategies by which people can modify and/or adapt to these potential changes. Assessments of risks and cost/benefit analyses can be conducted so that potential options for decision making can be based upon a truly comprehensive

Fig. 2 The CO_2 program.



understanding of CO_2-induced changes.

Carbon Dioxide Research aims to establish knowns and unknowns, reduce and specify uncertainties, increase data collection, and improve measurements and models directed at answering specific questions about the sources and sinks of CO_2, climate, and other possible effects.

Much of the current research is focused on defining and measuring fluxes of CO_2 among major sources and sinks of the carbon cycle. Research efforts also include estimates of global and regional changes in temperature and precipitation aimed at identifying which climate changes result directly from the effects of CO_2 (as differentiated from the many other factors that could have been involved). General circulation models are being used to determine how atmospheric CO_2-induced climate change may relate to the nonatmospheric components of the climate system, such as oceans, land, and the cryosphere. Preliminary results of studies with nonatmospheric-ocean models suggest that effects may be delayed a decade or more by the thermal inertia of the oceans. The photosynthesis, physiology, and water use of plants and trees are also being studied to provide a basis for predicting the responses of vegetation to rising atmospheric CO_2.

In 1977, recognizing the paucity of scientific data and the uncertainties surrounding our understanding of possible global climate change as a function of increasing atmospheric CO_2, DOE and several other federal agencies began a concerted effort to define the CO_2 issue. The DOE initiated a new research program, the first step being to convene a series of workshops and conferences. These workshops led to commissioned papers, which in turn became the basis for long-term research plans. A focused research program has, thus, been designed to develop the scientific knowledge base to aid in analyzing possible energy policy options related to potential CO_2 effects. The efforts of DOE and the other agencies are now being coordinated by the National Climate Program Office, established by the National Climate Program Act (P.L. 95-367) and administered by the National Oceanic and Atmospheric Administration. The DOE is the lead agency for investigation of CO_2. Other agencies involved in the program include the National Aeronautics and Space Administration, the U. S. Geological Survey, the Department of State, the Environmental Protection Agency, and the National Bureau of Standards. The major efforts of the Carbon Dioxide Research program are currently focused on the cross-hatched areas of the figure on page 14.

Additional information about this subprogram is available from Frederick A. Koomanoff, Director, Division of Carbon Dioxide Research, ER-12, Office of Basic Energy Sciences, Department of Energy, Washington, DC 20545.

Major BES Facilities

Basic research in most areas pertinent to the DOE mission requires highly complex equipment and facilities. As mentioned earlier, the construction and operation of such facilities is costly, but many research projects rely on their availability. Basic Energy Sciences currently operates a number of facilities that are unique in the United States and, in some cases, in the world. The major BES facilities are described and their functions discussed briefly in the following subsections.

High Flux Beam Reactor

Brookhaven National Laboratory, Upton, New York

The High Flux Beam Reactor (HFBR) produces high-intensity neutron beams for research in a wide variety of fields. Neutrons are used as probes by nuclear and solid-state physicists, chemists, and biologists. Neutron scattering techniques continue to yield information on the fundamental properties and behavior of materials and chemical and biological substances which cannot be obtained by any other means. The HFBR is one of two high-flux research reactors supported by DOE, both of which are world-class research reactors for neutron research.

Current research using the HFBR includes studies of:

- The structure and dynamics of magnetic materials by elastic and inelastic neutron scattering
- The dynamics of materials as they change phase by quasi-elastic neutron scattering
- Neutron irradiation effects on the physical properties of materials
- The molecular structure and dynamics of organometallic substances
- Small-angle neutron scattering of biological substances
- The lattice structure and dynamics in condensed matter systems
- Amorphous materials—short-range order and excitations
- The neutron spectroscopy of low-lying excited states in solids

The HFBR, which cost $12.5 million to build, went critical in 1965 and attained full power in 1966. Originally 40 MW, its power was increased to 60 MW in 1982. The reactor has a maximum thermal neutron flux of 1.1×10^{15} neutrons/cm^2-sec available for research. Several of the nine experimental beam ports are used by more than one scattering instrument; three are used for nuclear physics research, and the rest for neutron diffraction or scattering research. The reactor can also be used to irradiate samples through any one of seven different vertical access tubes. The in-core total flux is 2.4×10^{15} neutrons/cm^2-sec. The building that houses the reactor and ancillary equipment has floor space for experimental apparatus. A cold moderator facility, recently installed, establishes HFBR as the largest source of very low energy neutrons in the United States.

High Flux Isotope Reactor

Oak Ridge National Laboratory, Oak Ridge, Tennessee

The High Flux Isotope Reactor (HFIR) has a high thermal neutron flux designed for production of transplutonium elements. This facility is critical to the Transplutonium Production Program of DOE. In addition to producing transplutonium elements, HFIR has four ports to permit the extraction of neutron beams from the reactor core for experimental purposes. The high flux and experimental capabilities make HFIR a unique research reactor, important not only for isotope production but also for neutron scattering, nuclear chemistry, and radiation damage research.

Although the use of HFIR has changed direction over the years, with increased emphasis on neutron irradiation and beam research and radioisotope production for sales, transplutonium isotope production continues to be the major effort. With the shutdown of the General Electric Test Reactor, which was a commercial supplier of a variety of radioisotopes, HFIR provides substantial quantities of radioisotopes to the industrial community. These sales, at full cost recovery, have resulted in revenues to HFIR of about $600,000 to $800,000 annually.

The HFIR cost about $15 million to build and attained its operating power of 100 MW in 1966, with a thermal flux in the target area of 2 to 5×10^{15} neutrons/cm^2-sec. It has a unique, one-piece core, which is its fuel element; this core is about the size of a 30-gal drum and is replaced after about 3 weeks of operation. In addition to isotope production activities and in-core irradiations, there are twelve research stations at four experimental ports. Associated with the HFIR is the National Center for Small Angle Scattering Research, sponsored as a joint project of DOE and the National Science Foundation.

In FY 1983 total HFIR operating costs were about $6.7 million, of which about $1.0 million was defrayed by non-BES user research programs and radioisotope sales.

BES-supported research activities at HFIR in FY 1983 were at about $5 million. Other research at HFIR is supported by the Fusion and Fission Energy Programs, the Nuclear Regulatory Commission, and the National Science Foundation.

National Synchrotron Light Source

Brookhaven National Laboratory, Upton, New York

The National Synchrotron Light Source (NSLS) is a unique user-oriented facility for advanced multidisciplinary research with synchrotron radiation. At NSLS a wide range of research techniques are used by biologists, chemists, solid-state physicists, metallurgists, and engineers for basic and applied studies. Among the techniques are extended X-ray absorption fine structure (EXAFS), scattering, diffraction, topography, fluorescence, interferometry, gas phase spectroscopy, photoemission, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

The highly intense radiation emitted by electrons travelling in circular paths at very high energies is referred to as synchrotron light. Synchrotron light radiation from the NSLS is continuous in spectrum, stable, pulsed, and high in intensity, with the spectral peak related to the electron energy and radius of the circular orbit. Some applications of the interaction of synchrotron radiation with matter are:

- Studies of the state and behavior of gases
- Studies of the surface of solids
- Studies of metal atoms in biological systems
- Analysis of the atomic structure of microscopic samples
- Microscopy
- Research related to the miniaturization of computer chips

The NSLS, which began operating in 1981, includes two electron storage rings—an X-ray ring about 170 m in circumference, which provides 28 photon ports, each able to handle one or more experiments, and a vacuum ultraviolet (VUV) ring 44 m in circumference, with 16 photon ports. A common injector meets the high-current requirement (1.0 A) for both rings. The VUV ring has been used routinely for research since early 1984. It operates at 750 MeV and has achieved peak currents over 400 ma with average 100 ma lifetimes of more than 2 hours. The x-ray ring is in the commissioning stage. It has operated at 2.0 GeV with 70 ma, about 15% of the design current. Some initial experiments are being staged. The users of the NSLS facility include individual university researchers, national laboratory teams, and industrial researchers from such Fortune 500 corporations as IBM, Exxon, Bell Laboratories, DuPont, General Electric, and Mobil. The authorized construction cost for NSLS ($24 million) provided for the building, storage rings, and a limited amount of experimental equipment for four of the beam ports. Substantial additional instrumentation and equipment has been installed, with private industry committing more than $8 million.

Stanford Synchrotron Radiation Laboratory

The Stanford Synchrotron Radiation Laboratory (SSRL) is one of several national facilities for the utilization of synchrotron radiation for basic and applied research in chemistry, physics, biology, and materials science. The available synchrotron radiation is produced by the 4-GeV storage ring SPEAR operated by the Stanford Linear Accelerator Center (SLAC). The SSRL is a user-oriented facility that welcomes inquiries and proposals for experiments from qualified scientists.

The extraordinary properties of synchrotron radiation as a research tool have led to many very important scientific results including:

- Development of the Extended X-ray Absorption Fine Structure (EXAFS) technique as a powerful structural tool
- Many advances in surface physics based on the photo-emission technique, using high intensity tunable VUV radiation from 10 to 1000 eV
- Dynamic studies of conformational changes in biological systems, using time dependent x-ray diffraction and fluorescence lifetime techniques
- Development of anomalous diffraction as a broadly applicable tool of crystallography
- Results in other areas such as topography, lithography, and microscopy

CAPTION: The photograph is an aerial view of the 4-GeV storage ring spear and SSRL laboratories at SLAC. The SSRL is housed in two buildings on the spear ring. The building in the forefront houses the offices and three beam lines. The building on the opposite side of the ring houses another three beam lines and support facilities. The large double-peaked building inside the ring contains the storage ring control room and power supplies. Entering the ring tangentially from the right are the electron and positron injection lines. The cleared space in the forefront of the picture is the site of the new light assembly building being constructed under the SEP Program.

SSRL has many experimental stations in operation. These provide white radiation and monochromatic radiation over a broad spectral region from the visible through the ultra-violet and deep into the x-ray region to 40 KeV and beyond.

Synchrotron radiation is available in either dedicated or parasitic mode. Half of the time, the SPEAR ring is operated in high-current single-beam mode as a dedicated synchrotron radiation source. During the other half of the time, radiation is available during colliding beam runs for high-energy physics research. In colliding beam runs, radiation occurs in 200 to 400 picosecond pulses at a rate of 1.28 MHz.

During dedicated runs, the SPEAR energy that best satisfies user needs is selected; this is generally 2.6 to 3.7 GeV, with most operation near 3.0 GeV. The stored current is typically 75 to 100 mA. Most colliding beam operation is at or near 2.0 GeV, with stored electron currents of about 10 mA.

Synchrotron radiation, the electromagnetic energy produced by relativistic electrons in magnetic fields, has many unusual properties that make it a most effective experimental tool. The SPEAR spectrum extends from the infrared through the visible, UV, VUV, and deep into the x-ray region. As a continuum source, synchrotron radiation is unrivaled. For example, in the x-ray region, SPEAR provides five orders of magnitude more continuum radiation than the most powerful conventional x-ray generators in many experimental situations.

SSRL has six beam lines, most with multiple experimental stations.

Intense Pulsed Neutron Source

Argonne National Laboratory,
Argonne, Illinois

The Intense Pulsed Neutron Source (IPNS) is a dedicated user-oriented facility for advanced multidisciplinary research with pulsed neutrons, serving the physics, materials, chemical, and life sciences research communities.

Unlike reactor sources, this machine provides high fluxes of neutrons in bursts that are synchronous with the 30 Hz frequency of the proton accelerator. High-energy protons from a proton synchrotron impinging on a heavy metal target produce bursts of spallation neutrons. The resulting pulsed beams of neutrons, exploited using time of flight techniques, have the following characteristics:

- High peak intensity thermal neutrons
- High peak intensity epithermal neutrons
- Pulsed delivery for investigating time-dependent phenomena, such as following shock waves, heat pulses, or laser flashes

In materials research, pulsed neutrons can be used to study:

- Static and dynamic properties of liquids and amorphous solids
- Defects, voids, and aggregates in materials
- Structure and dynamics of polymers and biological material
- Magnetic, crystallographic, and electronic changes
- Phonon structure and magnetic excitations in solids
- Surface phenomena and superconductivity
- Radiation damage studies at cryogenic temperatures

The IPNS, which began operation in FY 1981, has the following operating characteristics:

Proton current	8 μA
Protons/pulse	2×10^{12}
Proton energy	500 MeV
Repetition rate	30 Hz
Peak thermal flux	3×10^{14} neutrons/cm^2-sec
Peak epithermal flux (1 eV)	10^{15} neutrons/cm^2-sec
Time-average fast flux (0.1 MeV)	2×10^{12} neutrons/cm^2-sec

The neutron scattering assembly has seven spectrometer stations, and the radiation effects assembly includes two cryostat stations for investigations at 4°K. Six additional facilities are available for special experiments with, for example, solid He^3, polarized neutrons, and ultracold neutrons, and for high-temperature irradiations. During the initial experimental period in 1982, 29 of the 38 experiments performed were by outside users.

The authorized construction cost for IPNS ($6.4 million) provided for beam transfer from the proton synchrotron and construction of the spallation target area. In addition, $2.4 million was provided to upgrade the experimental capability with a variety of spectrometers, detectors, and computer interfaces.

Combustion Research Facility

Sandia National Laboratory, Livermore, California

The Combustion Research Facility (CRF), which cost $10.3 million, provides a range of instrumentation not available in other laboratories and, thus, provides a unique capability to outside users for combustion research. It receives considerable use by non-DOE groups. The focus of the laboratory is on laser diagnostics of combustion systems, but a variety of burner systems and special facilities are available, including those for research on coal combustion and internal combustion engines. The staff at CRF provides users with technical support covering such diverse fields as chemistry, fluid dynamics, computer modeling, and pure and applied spectroscopy. The CRF research staff also has the necessary scientific strengths to serve the DOE combustion program's research objectives—maximizing the efficiency of processes while minimizing the production of undesirable pollutants. Examples of research that is carried on at CRF include:

- Detection and measurement in flames of short-lived reactive intermediates in key combustion reactions
- Modeling and improvement of the use of ammonia to reduce NO_x emission from combustion processes
- Laser velocimetry to study turbulence effects in an internal combustion engine
- In situ laser diagnostics of the interactions of materials surfaces with flames

The CRF, a building with fourteen individual research laboratories, four special laser laboratories, and a variety of support laboratories, was dedicated in early March 1981. On demand, laser output can be beamed to any one of the individual research laboratories for use in a large variety of experiments.

High-Voltage and Atomic Resolution Electron Microscope Facilities

High-Voltage Electron Microscopes (HVEM) are invaluable for energy-related research important to, e.g., fission and fusion (radiation damage), automotive (high-strength steel and high-temperature ceramics for automotive turbines), fossil (corrosion), and solar (photovoltaics) technologies. The microscopes are also important for general research, and each institution having one has developed or is developing a sizeable outside user group of academic and industrial scientists.

The HVEM is useful for transmission electron microscopy of heavy metals, studies that must use "thick" samples to avoid surface effects, and studies of brittle materials, such as ceramics, which are difficult to prepare in thin form. Also, high-voltage machines are necessary for materials studies incorporating special environments and for in situ radiation damage studies. It is possible to "see" damage as it is being produced. The only other federal agency supporting MeV microscopes is the National Institutes of Health, which has several machines for medical and biological research.

Basic Energy Sciences supports three facilities with HVEM's and the atomic resolution microscope (ARM), which came on-line in 1983.

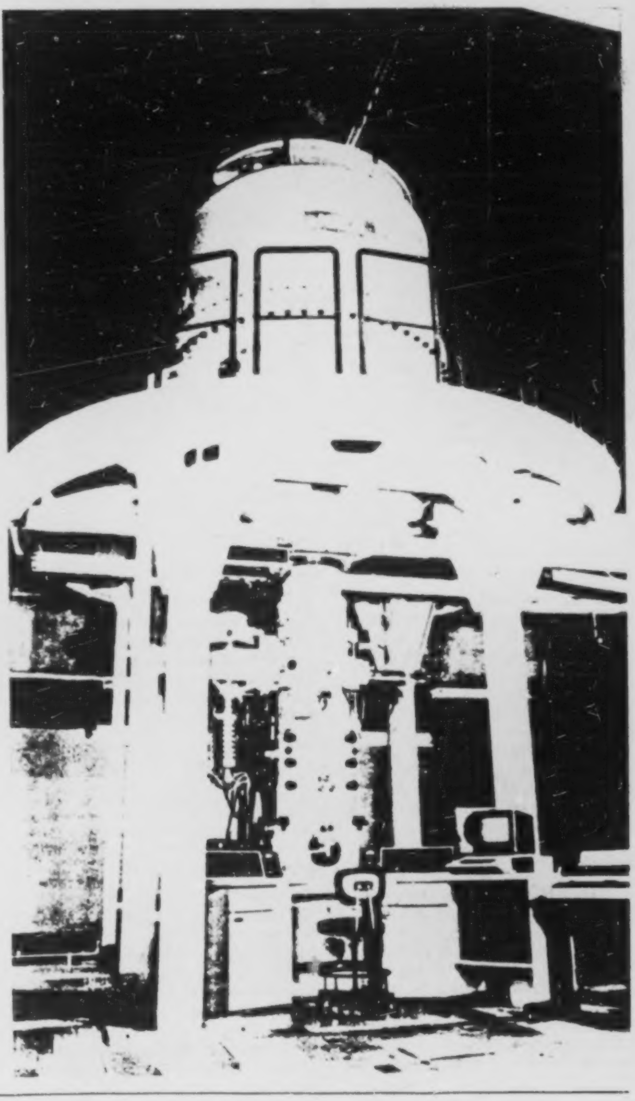
National Center for Electron Microscopy, Lawrence Berkeley Laboratory, Berkeley, California

On September 30, 1983, the National Center for Electron Microscopy (NCEM), which cost $8.0 million dollars, was dedicated. The Center's dedication culminated nearly 9 years of research, development, and construction. NCEM contains the most advanced electron microscopes in the world and has as its centerpiece the only atomic resolution electron microscope (ARM) in the United States. Besides the ARM, other available microscopes are a Hitachi HU-650, Kratos EM-1500, and JEOL 200 CX.

The JEOL JEM-ARM-1000 was specifically designed for ultimate performance in the high-resolution imaging mode. Attention has been given to the potential problem of specimen sensitivity to the electron beam at higher accelerating voltages, and a microprocessor-controlled height variable goniometer has been incorporated so that the microscope will operate with minimum aberration over its entire voltage range (400 to 1000 KeV). At its maximum voltage (1 MeV), the ARM has a point-to-point resolution of 1.7 Å. At higher lens excitation values, the microscope can be run in condenser-objective mode; this enables convergent beam electron diffraction (CBED) patterns to be taken from the same specimen areas imaged in high resolution.

For increased stability, the stage configuration on this machine is top entry, with standard 3-mm-diameter specimen cartridges; it is coupled to a microprocessor for precise stage manipulation. The microscope uses LaB_6 filaments for additional brightness, and the camera accepts 50 film cassettes.

The Kratos EM-1500 High Voltage Electron Microscope is designed primarily for dynamic in-situ studies, but it can also resolve structures at the 3 Å level. It is the first electron microscope with a maximum acceleration voltage of 1.5 MeV to be built by Kratos. As such, it provides accelerating voltages of 1200 to 1500 KeV, which are not available elsewhere in the United States. To achieve the higher accelerating voltage, the number of stages of the Cockcroft-Walton generator was increased to 9 and the SF_6 insulating gas pressure was increased to ~90 psi. Conditioning of the accelerator tube is carried out at 1.6 MeV. The accelerating voltage actually can be set at 150 or 200 to 1500 KeV in 100-KeV increments. The microscope is equipped with both a top-entry stage for high resolution studies and a side-entry stage for general, dynamic in-situ, and environmental cell studies. Several different specimen stage rods are available (see table on p. 22), and this inventory will be increased as needed.



SPECIMEN STAGES FOR EM 1500

Type	X-Tilt	Y-Tilt	Temperature
Double tilt, cartridge type	±45°	±45°	Ambient
Single tilt, cartridge type*		±45°	Ambient
Double tilt, furnace type	±30°	±30°	Ambient to 850
Single tilt, furnace type*		±25°	Ambient to 850

*For use with Environmental Cell at pressures up to 1 atmosphere.

A support instrument to the ARM, the JEM 200-CX is well-known for its high-resolution performance. This machine, which is equipped with an ultrahigh resolution goniometer (top entry), has a maximum operating voltage of 200 KeV with a point-to-point resolution of about 2.4 Å. Specimens for this microscope are restricted to 2.3 mm in diameter to fit into the ultrahigh resolution pole piece.

The fourth microscope at LBL is the Hitachi HU-650. It has an accelerating voltage that is continuously variable between 200 and 650 KeV, but it is calibrated for, and most conveniently used at, three fixed voltages, 300, 500, or 650 KeV.

The resolution limit of this instrument is not high—about 20 Å—but it is adequate for some studies, exploratory experiments, and many hot stage or environmental cell experiments.

High Voltage Electron Microscope-Tandem Facility, Argonne National Laboratory, Argonne, Illinois

The High Voltage Electron Microscope (HVEM)-Tandem Facility is operated as a national materials science resource available to qualified scientists in the United States. The facility provides unique combinations of the techniques of a high-voltage electron microscope, ion implantation/bombardment, and ion-beam analysis. In addition, the HVEM/ion-beam interface permits direct observation of the effects of electron and ion bombardment on materials in the microscope. The ion-beam interface is an instrumental beam transport that connects the 2-MeV tandem and the 300-KeV ion accelerators to the HVEM. Current experimental studies using the HVEM represent a wide range of materials research from universities, national laboratories, and industry. Work includes programs in mechanical properties, corrosion and oxidation, radiation damage, and general defect analysis.

The principal components of the HVEM-Tandem Facility are a Kratos 1.2-MeV high-voltage-transmission electron microscope with ion-beam interface, a National Electrostatics 2-MeV tandem-type universal ion accelerator, and a Texas Nuclear 300-KeV ion accelerator. These two accelerators together provide ion beams of essentially all elements from ~10 KeV to 8 MeV. Contiguous support facilities for the microscope include two darkrooms, a specimen-preparation laboratory, an instrument laboratory, and a preparation laboratory for mechanical work shared with the accelerator facility.

The high-voltage electron microscope is an improved Kratos/AEI-EM7 with a maximum voltage of 1.2 MeV and a demonstrated lattice resolution of 3.5 Å. In addition to a 33° ion-beam access tube, the microscope contains a number of unique features. These include a negative ion trap, an ion-pumped specimen chamber, two independently adjustable dark-field conditions, and a 100 to 1200-KeV continuous-mode voltage selection from the control desk. The electron beam dosimetry system consists of a retractable Faraday cup above the specimen and a movable cup above the fluorescent screen to probe the current density profile of the beam. Special specimen rods for viewing and for measuring the intensity of the ion beam within the microscope also are available. Observations can be made at temperatures between 10 and 130°K in high-vacuum conditions. Observations in gaseous atmospheres at pressures of up to 2.5×10^4 Pa can be carried out between ambient temperature and 1300°K using a gas reaction cell inserted into the specimen chamber. This HVEM is equipped with the Harwell-design camera and has a capacity of 48 plates and a video monitoring and recording system.

The National Electrostatics Type 2UDHS 2.0-MeV Tandem Accelerator is equipped with an internal and two external negative sources for He$^-$ and metal ions, respectively. The machine can generate ions of all stable isotopes in the periodic table. The accelerator can be operated in conjunction with the HVEM or separately for ion implantation/bombardment and ion-beam-analysis studies. Typical ion-beam currents will range from ~10 A for protons to 0.1 μA for $^{204}Pb^+$.

There is also a 300-KeV ion accelerator that has been equipped with sources for metal and gaseous positive ions. This accelerator can be used in conjunction with the ion-beam interface when lower-energy ions are required or to deliver ions into two of the target chambers of the Tandem system for ion implantation studies. The 300-KeV accelerator cannot be used when ions from the Tandem are passed into the ion-beam interface.

Shared Research Equipment Program, Oak Ridge National Laboratory, Oak Ridge, Tennessee

The Shared Research Equipment program (SHaRE) is a collaborative program in which personnel at Oak Ridge National Laboratory work with scientists from other institutions. It is the third facility having an HVEM. The purposes of the program are to provide university and industrial researchers with access to equipment for microstructural analysis which is not available at their home institutions and, in so doing, to facilitate additional laboratory research that would not otherwise be accomplished. The laboratory staff shares with visitors responsibility for both completing the project and ensuring publication of the results.

A number of major instruments are available to collaborators. Nuclear microanalysis and Rutherford backscattering analysis are performed in two separate systems, and four variously equipped 120-KeV transmission electron microscopes are in service. A Hitachi 1-MeV HVEM is equipped for environmental and mechanical deformation investigations. Two Auger analysis systems, one with scanning capability, also belong to the equipment pool in the SHaRE program.

Oak Ridge Electron Linear Accelerator

Oak Ridge National Laboratory, Oak Ridge, Tennessee

The Oak Ridge Electron Linear Accelerator (ORELA), a facility of continuing importance in the development of fission and fusion energy technologies, is used for measurements of neutron cross sections over a whole range of thermal energies, from 0.02 eV to 80 MeV. These cross sections are needed to design and operate nuclear fusion and fission power reactors and to study some aspects of nuclear reaction mechanisms and nuclear structure. At present cross sections are best measured by repetitive, intense neutron pulses and the short-burst performance of ORELA. Energy-dependent neutron cross section and related measurements of almost every variety are made with this facility. The ORELA was upgraded several years ago with a new electron gun and klystron prebunching system to increase the effective neutron output.

The ORELA, which was built in 1969 at a cost of $10 million, provides 22 A peak currents of 100- to 170-MeV electrons at burst widths from 3 to 24 nsec at the rate of 25 to 1200 pulses/sec. The electrons impinge on a target material producing the desired neutrons. At an average power of 50 kW, 10^{14} neutrons/sec, time averaged, or 4×10^{18} neutrons/sec, peak, are produced. The design of ORELA, which includes eleven flight paths radiating from an evacuated target room, makes possible simultaneous use by many experimenters, a feature that greatly increses the total output and cost-effectiveness of the facility.

5-MeV Dynamitron Accelerator

Argonne National Laboratory,
Argonne, Illinois

The Argonne Dynamitron accelerator provides intense, highly collimated direct-current beams of fast atomic or molecular ionic projectiles for use in experiments in atomic physics, nuclear research, and the irradiation of materials. In operation since 1968, it has been steadily improved over the years. It is a powerful, versatile, and reliable facility that also includes computer systems for control and data acquisition.

Present applications of the accelerator include studies of the interactions of fast molecular ions with matter, determination of molecular ion structures, beam-foil spectroscopy, and ion channeling in crystals. Nuclear research includes weak interaction studies, measurements of parity violation in nuclei, quark searches, and measurements of the cross section for reactions between light nuclei. The materials research is centered on damage studies related to the first-wall problem in fusion reactors.

A valuable feature of the machine is that a broad range of positive-ion projectile species can be accelerated and analyzed magnetically. There are six fully instrumented beam lines, including one with a unique capability for experiments requiring extremely high angular resolution and one equipped for simultaneous dual-beam irradiations with a magnetically analyzed beam from a neighboring 20-MeV Van de Graaff accelerator merged with the Dynamitron beam. The accelerator voltage can be varied smoothly between 0.3 and 5.0 MeV. Monatomic positive-ion beams of most of the elements are readily produced, as are molecular-ion beams, including such complex projectiles as $C_6H_6^+$. Most beams are available at the microampere level, and some (e.g., hydrogen and deuterium beams) at the milliampere level, continuously or in a pulsed mode down to a few tenths of a nanosecond and at repetition rates variable up to 8 MHz.

Calutrons—Electromagnetic Isotope Separations Facility

Oak Ridge National Laboratory,
Oak Ridge, Tennessee

The electromagnetic isotope separations facility at Oak Ridge National Laboratory (ORNL) enriches stable isotopes, selected radioactive isotopes, and heavy-element isotopes for use in research and development and in commercial activities. It consists of very high current mass separators, known as Calutrons, which were originally designed and built under the Manhattan Project during World War II. The Calutron facility is a unique national asset; the USSR is the only other nation possessing such a facility. Many other countries have laboratories in which isotopes are enriched, but these facilities are usually of limited size and the isotopes are used for specific purposes. Research and development directed toward increasing both the throughput and the isotopic purity of the products is also conducted at ORNL. The Isotope Sales Office distributes the isotopes in two ways: Multigram quantities of enriched samples from the Research Materials Collection are loaned to members of the DOE research community at a nominal fee for nondestructive research, and enriched isotopes are sold to other research and commercial organizations on a cost-recovery basis.

The facility consists of two "tracks" containing 62 separator tanks. Eight tanks are reserved for chemically hazardous and radioactive elements and 44 for stable isotopes. Of these, 30 comprise the stable isotope track. The remaining ten tanks can be used to separate either radioactive or stable isotopes. The horizontal magnetic field of the stable isotope track is subdivided into four segments by magnetic shunts that extend from one side of the track to the other. The resulting three banks of eight separators and one bank of six separators can be used independently. If the magnetic field in each separate segment is excited, it is theoretically possible to enrich the isotopes of four elements simultaneously in the 30 Calutrons. A recent operational improvement has established that, for cases where the isotopic mass ranges of several elements overlap, the isotopes of these elements can be separated simultaneously in one magnetic segment.

When feed material, in either elemental or compound form, is introduced into a Calutron, it is either directly vaporized or heated with chemical treatment to form a volatile species. This vapor is then introduced into an arc discharge, where it is ionized in the high-current source. The ionized particle is extracted from the ion source, accelerated, and magnetically focused. The focused individual isotopic beams are intercepted by collectors constructed of carbon, copper, or aluminum. After a run, the duration of which may be fifty to several hundred hours depending on the element, the collectors are removed from the separator, and the material is extracted, chemically purified, assayed, and placed in the inventory.

Since each element or compound has unique operating characteristics, it is difficult to generalize about the throughput capability of the facility. Typical beam currents are between 10 and 100 mA, with an average of 25 to 50 mA. As a rule of thumb, one separator can provide approximately 0.1 mole of an element per day of operation. This figure is multiplied by the natural isotopic abundance to determine the yield for a particular isotope. Isotopic purity depends on the natural isotopic abundance of the isotope required and the abundance of its nearest neighbors. The products of one separation can be recycled to obtain a significantly higher isotopic assay in a two-pass process.

Materials are available from the Research Materials Collection (RMC) for loan to U. S. scientists for use in nondestructive experiments and to non-U. S. scientists under restrictive conditions (e.g., the experiment must be of direct relevance to the DOE technology programs, such as the use of RMC samples within the European community for the study of neutron cross sections). Such loans are usually made only on the strong recommendation of the U. S. Nuclear Data Committee.

Materials are sold from the sales inventory to anyone on a first-come, first-served basis. Up-to-date information on the electromagnetically enriched isotopes, their chemical form, percent enrichment, price per milligram, and availability can be obtained from E. Newman, Operations Division, ORNL, P. O. Box X, Oak Ridge, TN 37830.

Transuranium Processing Plant

Oak Ridge National Laboratory,
Oak Ridge, Tennessee

The Transuranium Processing Plant (TRU) was built to recover radioactive transuranium elements from irradiated targets and to serve other chemical processing and fabrication needs of the Transplutonium Production Program of the Atomic Energy Commission. It is not a research facility for BES, but it provides unique chemical processing capabilities for highly radioactive actinide materials. Research in nuclear chemistry and physics and nuclear technology, especially as related to fission energy development and to fundamental behavior of the actinide radionuclides that pose significant problems in nuclear waste treatment and isolation, is supported by TRU activities. A nuclear energy program "user" group currently in residence at TRU operates the Solvent Extraction Test Facility, which is part of the ORNL Consolidated Fuel Reprocessing Program.

Samples ranging from hundreds of grams of curium-244 to picograms (10^{-12}) of fermium-257 have been provided by TRU, and research quantities of a variety of transuranium isotopes prepared at TRU have contributed to our understanding of the chemical, physical, and nuclear properties of the actinide elements.

The TRU, built at a cost of $8.8 million, began "hot" operation in 1966. It contains seven hot cells, each equipped to carry out remotely one or more separate procedures for chemical separation, purification, fabrication, or analysis of highly radioactive materials.

In addition to its use for the nuclear energy program's solvent extraction research and development, the facility also contributes to DOE's isotope production and sales activities.

Program and Budget Trends

Basic Energy Sciences (BES), as the program responsible for fundamental, longer term, research supportive of the mission of the Department of Energy, is committed to continuing studies in the physical and related sciences. It has funded and conducted creative research programs and managed complex facilities for DOE and its predecessor organizations since the 1940s, a period of unparalleled scientific growth and achievement.

Basic Energy Sciences long range research complements and undergirds the applied research and development activities of DOE's technology programs. The BES program is not likely to advance DOE's short-term goals, nor is it supposed to. Its major product is fundamental knowledge relevant to energy exploration, production, conversion and use. This new knowledge becomes part of the body of information upon which the applied technologies rest. While research to broaden the technology base needed for identified energy technology options is extremely important, even more important, to constantly improve our science base, is our need for basic research unfettered by preconceived notions of what technologies will be important several decades from now. It is from such basic research and its generation of new ideas and concepts that new, currently unidentified options may emerge.

Basic Research is a necessary investment in the future and continuous, uninterrupted research programs are invaluable to the nation in providing a knowledge base on which to build. Because of its experience, diversity, and unique capabilities, BES continues to be able to respond to growth and new directions in national goals and missions.

Table 1 Office of Basic Energy Sciences Budget

	FY 1983 10^6 dollars	FY 1984 10^6 dollars	FY 1985 10^6 dollars
Operating Expenses (by subprogram)			
Materials Sciences	108.2	125.1	133
Chemical Sciences	70	75.5	79.5
Nuclear Sciences	30.6	37.9	40.3
Applied Mathematical Sciences	13.9	14.7	35.1
Engineering and Geosciences	17.2	19	26.7
Advanced Energy Projects	8.3	9.1	10.6
Biological Energy Reseach	9.5	10.6	12.5
Carbon Dioxide Research	9.1	12.5	13.4
Program Direction	3.2	4	3.8
Subtotal	270	308.4	354.9
Capital Equipment	18.2	24.3	31.1
Construction	3.4	17.2	50
Total	291.6	349.9	436

During the decade from 1973 to 1983, BES experienced a significant expansion in its research responsibilities to include knowledge required by non-nuclear energy technologies. Towards the end of this period, several major construction projects were reaching fruition and the BES budget growth rate increased, primarily to meet the special needs associated with the operation of the newer facilities and for new construction projects. The budget for FY 1984 is approximately $350 million (Table 1) of which $24.3 million, about 7%, is for capital equipment, and the fraction of the FY 1984 budget appropriation designated for construction rose to 5%.

Some changes in responsibility occurred during FY 1984. The Division of Engineering, Mathematical, and Geosciences was restructured with the Applied Mathematics Sciences management responsibility being transferred to a newly formed office under a director of Scientific Computing. The budget for Applied Mathematical Sciences continues to be under BES.*

Research support for Heavy Ion Fusion Research which previously had been conducted under the Defense Program was included in the Nuclear Sciences subprogram at a level of $5 million. Also in FY 1984, several new construction projects were undertaken, one for facilities at LBL to comprise a new Center for Advanced Materials Research, and two others, at the initiative of the Congress, to provide updated, modern buildings for research on university campuses.

Figure 3 presents a breakdown identifying the major performers who carry out the Basic Energy Sciences program. About 69% of the program is conducted at the national laboratories including Lawrence Berkeley Laboratory (LBL) and Ames Laboratory, 26% at universities throughout the country, and the remainder elsewhere, including nonprofit institutions and industry. Plans are to maintain the university portion of the program at about 26%, not including Ames Laboratory and Lawrence Berkeley Laboratory. These two major laboratories, which are colocated with universities (Lawrence Berkeley at the University of California, Berkeley, and Ames at Iowa State University), receive almost one-fifth of the BES support going to national laboratories. If they are included with the universities, that portion of the program rises to 39%, with a corresponding decrease under national laboratories. The research supported by BES at Ames and LBL is conducted almost entirely by faculty members and graduate and postdoctoral students.

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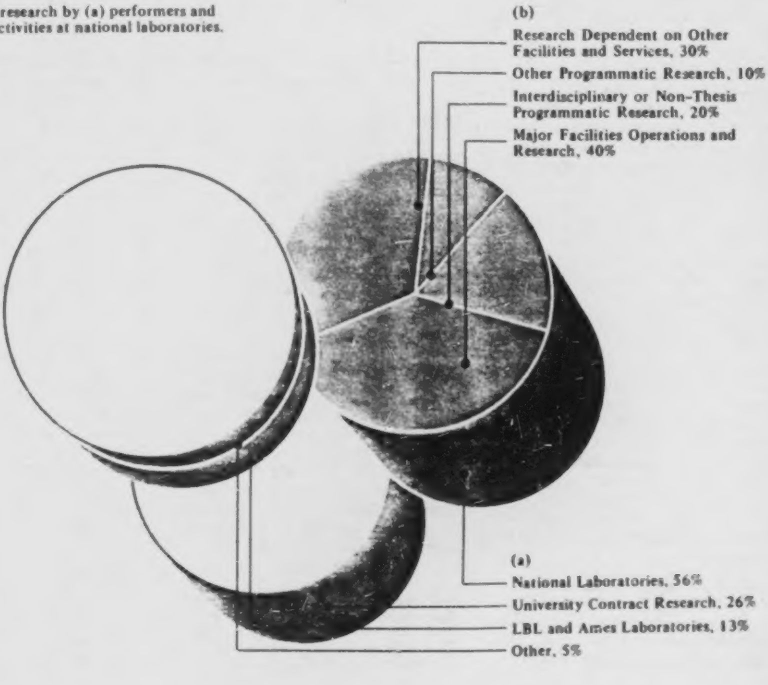
*Information on the Applied Mathematical Sciences is available from Dr. James F. Decker, Director of Scientific Computing, ER-7, Office of Energy Research, DOE, Washington, D. C. 20845.

Of the funding going to national laboratories, about 90% is for activities uniquely dependent on the facilities and services at the specific laboratories supported. The operation of major scientific facilities continues to require a large commitment of BES funds. Operating costs for facilities for FY 1984, exclusive of the costs of research done at the facilities, are projected at $55 million; they are expected to rise to nearly $70 million in FY 1985.

The future for BES continues to be more and more challenging as the frontiers of science expand. Current trends are toward greater use of the major facilities, by both DOE and "outside" researchers, and strengthening of research in the areas of science dealing with:

- Surfaces--modification, interfaces, reactions at surfaces
- Solids—properties and structure, including grain boundaries, condensed matter theory, atomic transport, amorphous materials, structural ceramics
- Plants—genetics, response to stress, photochemistry
- Geothermal energy resources—occurrence, characterization, chemical and thermal properties
- Multiphase systems—transport properties, chemical behavior, etc.

Figure 3 Breakdown of research by (a) performers and (b) nature of research activities at national laboratories.



Experiments with, for example, phenomena involving extremely short time periods, vanishingly small concentrations of reacting species, entities with only transient existence, and measurements under extreme conditions of temperature and pressure point out the necessity for constantly improving equipment. Examples of BES's efforts to meet these kinds of challenges include the new Atomic Resolution Microscope which came on line in 1983, and the ever increasing efforts to exploit synchrotron radiation and advanced neutron sources to increase our understanding of the atomic structure of materials.

Despite increasing costs and demands for constantly improved equipment and installations, the unique research programs and facilities supported by BES must be maintained, improved and expanded. The knowledge base they create is vital to improving or developing new energy technologies.

SOME EXAMPLES OF ACCOMPLISHMENTS

UNDER THE BASIC ENERGY SCIENCES

PROGRAM DURING 1984

FEBRUARY 1, 1985

Some Examples of Accomplishments Under the Basic Energy Sciences Program during 1984

February 1, 1985

The Basic Energy Sciences Program supports about 1200 research projects. The following selections do not fully reflect the full range of activities under the program; they are, however, examples of how basic research can contribute to solving a wide variety of energy problems.

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1. Metallic Glasses Now Synthesized Without Ultrarapid Quenching

Metallic glasses differ in structure and properties from metals. Metals normally have a crystalline structure with atoms in periodic arrays called lattices. In contrast, atoms in glassy metals do not form periodic arrays; their distribution is random. Originally devised a quarter of a century ago, the technique to produce amorphous or glassy metals required cooling the molten metal about one hundred thousand times faster than had previously been possible. Rapid cooling was the only way to prevent mobile atoms in the molten metal from rearranging themselves into crystal lattices. Recently it has been discovered that metallic glasses can be synthesized at low temperatures without quenching by directly introducing certain rapidly diffusing species into crystalline materials. Systems studied so far include hydrogen diffusion in some intermetallic compounds, gold diffusion in lanthanum, nickel diffusion in zirconium metal, and others. The common process in all of these systems is that one of the elements, viz., hydrogen, gold, and nickel in the above examples, diffuses very rapidly in the other at low temperatures. The rapidly diffusing species induces a phase instability which, because of the low temperatures, results in an amorphous structure rather than a crystalline structure.

Since metallic glasses have normally been produced by rapidly quenching liquid streams, metallic glasses actually have been limited in physical shape to very thin films or ribbons. Thus, despite their enhanced physical and mechanical properties over normal crystalline materials, applications of glassy metals have been limited to only those where such films or ribbons can be used. This new discovery thus has at least two significant implications.

First, from a scientific point of view, the discovery that equilibrium crystalline materials can be induced to transform to nonequilibrium amorphous materials is an exciting development. Second, it portends the possibility of preparing bulk (as opposed to thin ribbon) metallic glasses, thereby making metallic glasses with their enhanced magnetic and other properties accessible for a wider range of applications.

(California Institute of Technology, W. L. Johnson)

2. Stress Corrosion Cracking in Ductile Metals Explained By Localized Brittle Cracking and Altered Surface Layers

It has been experimentally observed that stress corrosion cracking (SCC) proceeds up to one thousand times more rapidly in ductile metal alloys than predicted using current theories. The discrepancy has been explained on the basis of localized brittle cracking which does not involve hydrogen, but which involves altered surface layers. This new mechanism was found in experiments on stress corrosion cracking of brass; the experiments coupled novel electrochemical and mechanical testing and nondestructive evaluation techniques and demonstrated that each increment of crack growth is accompanied by acoustic emission and a series of current transients. Molecular dynamics modelling, using two dimensional computer simultations of a crack in brass under conditions corresponding to those determined experimentally, corroborated the localized brittle cracking explanation.

This definitive delineation of a new brittle cracking mechanism in stress corrosion cracking both demonstrates that altered surface layers can change the fracture mode from ductile to brittle in normally ductile metals and resolves heretofore controversial experimental results obtained for some ductile metals.

(Brookhaven National Laboratory, K. Sieradzki, R. C. Newman, and H. S. Isaacs)

3. Ductility of New High Temperature Alloys Improved by Controlling Grain Boundary Chemistry

Nickel aluminide is an intermetallic compound that, until now, has been considered intrinsically brittle. Ductility levels useful for structural applications of nickel aluminide, however, have been observed and their occurrence has been definitively related for the first time to segregation of boron at boundaries between adjacent crystals in polycrystalline aggregates. The grain boundary concentrations of boron, aluminum, and sulfur in nickel aluminide have been measured using state of the art surface analytical spectroscopy techniques. The microchemistry data have been correlated with the macroscopic ductility of the material and the results are clear. Tensile ductility increases with increasing boron levels and decreasing sulfur and aluminum levels. Of particular importance, grain boundary segregation of boron is favored over sulfur when both are present in the alloy, so that conventional processing of materials in which minute levels of sulfur remain can be used.

This scientific result has major implications for alloy design. A new high-temperature oxidation resistant material, better than present superalloys, has been developed which can be produced by conventional casting and forming methods of alloys with modestly tightened composition limits. In the long term, understanding grain boundary microchemistry and relating it to the ability of grain boundaries to accommodate deformation without fracture underpins the development of all alloys. Brittle intergranular failure is the most significant failure mode for alloys in very long-term high-temperature service.

The potential of this aluminide has already been recognized by an IR-100 award as well as industrial interest in producing this material.

(Oak Ridge National Laboratory, C. T. Liu and C. L. White)

4. Advanced Electron Microscope Machines Holes and Slots in Thin Films to Atomic Dimensions

A novel machining method exploiting directed electron beam processing has been developed for boring holes and cutting slots in thin films with dimensions corresponding to those of ten atoms. This unique development permits machining to a dimension one thousandfold smaller than obtainable with commercial practice. This accomplishment was achieved by the use of a special electron source in a state-of-the-art electron microscope which focusses a very small, extremely high power electron beam on materials. Normally, the power level is low so that the material can be examined in the microscope. Above a threshold level, however, machining occurs in some materials, in particular, the aluminum oxides studied in this work.

This accomplishment has both scientific and technological importance. The fundamental behavior of atomic-dimension structures can be studied in a regime not heretofore accessible, namely, where the dimension of the specimen is smaller than critical distances controlling properties in bulk specimens. Wholly new technological vistas are opened up by this result--but new manufacturing concepts rather than refinement of current ones will be needed to exploit it. One potential application is the development of computer memories with storage densities one millionfold greater than presently possible, which will permit an enormous increase in complexity of problems to be studied. This new capability is possible only with advanced electron microscopes, and a patent application has been filed.

(University of Illinois, M. E. Mochel, J. A. Eades, C. J. Humphreys, M. Metzger, J. I. Meyer, J. M. Mochel)

5. Nuclear Magnetic Resonance Technique Broadened to Applications in Zero Magnetic Field

An important new use of nuclear magnetic resonance (NMR) as an instrument for science, technology, and medicine has been developed. NMR has been relatively weak in providing structural information on solids--e.g., how a material like a catalyst or a new alloy is constructed. With an amorphous substance like glass, or a polycrystalline one like zeolite catalysts, a broad, relatively featureless spectrum that contains little or no structural information is obtained because each "crystallite," or individual grain, of the substance has its own random orientation to the magnetic field. The new method developed, called "zero field NMR", cycles the sample between high magnetic fields and zero field. The extra resolution is achieved by measuring the spectra at zero field and allowing the nuclear spins themselves to act upon each other. With this resolution, the NMR spectrum of a powder becomes crystal-like, with clear, definite peaks, while amorphous materials have broad resonances characteristic of their short range order.

Zero field NMR promises to extend NMR to the analysis of such important industrial and biological materials as catalysts, plastics, and human tissue.

(Lawrence Berkeley Laboratory, A. Pines, D. Weitekamp and coworkers)

6. New Conceptual Basis Improves Prediction of Deformation Behavior of Metals

Combined theory and experimental measurements on large deformations (plasticity) of metals has led to a new "crystallographic" basis for deriving quantitative stress-strain relationships for polycrystalline metals. The conceptual difference between the old and new models for large strain plasticity of metals is significant--the new approach considers highly elongated grain shapes and favored orientations of planes in each grain with respect to local deformation, which is physically more realistic than earlier models which did not consider either grain shape or crystallographic orientations. Constitutive relations obtained with the crystallographic basis give substantially improved agreement between predictions of behavior and experimental results for brass and aluminum, particularly for loading conditions which are complex or involve changes from one stress state to another. In addition, the orientation of the crystal lattice in each grain of the aggregate was correctly predicted for the first time, confirming the physically realistic nature of the new model.

The validity and physical basis of the new model provide two improved capabilities heretofore governed by phenomenological models and empirical "rules." First is the ability to accurately extrapolate beyond an existing data base which must be obtained experimentally and, for complex conditions, at great expense. Second is the ability to use this extrapolation capability to predict failure criteria during metal working operations and thus avoid costly failures.

(Los Alamos National Laboratory, U. F. Kocks and M. G. Stout)

7. Advanced Neutron Scattering Techniques Developed for Studies at Very Low Temperature (.0027°K) and for Hydrocarbon Investigations

Both steady-state nuclear research reactors and spallation neutron sources are providing advanced capabilities in the effort to discover new properties of materials utilizing the unique capabilities of the neutron as a probe of matter. Using a steady-state reactor, nuclear ordering in praseodymium copper ($PrCu_2$) and holmium vanadate ($HoVO_4$) was observed for the first time at temperatures as low as 2.7 thousandths of a degree (.0027°K). These measurements were made possible by the use of a cryogenic dilution refrigerator together with a superconducting magnet which allowed these extremely low temperatures to be reached. At these temperatures, approaching absolute zero, fundamental properties of condensed matter, where atomic motion is nearly totally eliminated, can be obtained. This kind of information is important not only for the new properties discovered, but also for insights into the potential design of new materials with unusual properties. This experiment was part of a joint U.S.-Japan effort at Oak Ridge National Laboratory.

Utilizing the higher energy (epithermal) neutrons available from a spallation neutron source, new inelastic neutron scattering results were obtained from a series of hydrocarbons. Vibrational modes in this new high energy range were measured in butane and provided new structural information about that important hydrocarbon. The exploration of vibrational properties of hydrocarbons in this heretofore inaccessible energy range, gives new information that is important to advanced oil well logging diagnostics in the exploration of petroleum. In addition, the measurements provide new fundamental information about the hydrocarbons themselves. These experiments were part of a joint effort by Argonne National Laboratory and Schlumberger-Doll scientists.

(Oak Ridge National Laboratory, R. M. Moon and R. M. Nicklow; Argonne National Laboratory, D. L. Price; Schlumberger-Doll, W. Nelligan; Japan, S. Kawarazaki)

8. Ceramics Found to be Ductile Under Isothermal Forging Conditions

Two commercial glass ceramics have been found to be extremely ductile when mechanically tested at elevated temperatures under conditions that simulate isothermal forging. Each of these two materials contains a viscous glassy phase at grain boundaries at the testing temperatures of 1050° to 1150°C; the viscosity of the glassy phase is high in one and low in the other. The stress state, strain rate, and temperature were chosen so that fundamental information for an actual isothermal forging process could be obtained. The experimental results show that: (1) both materials are essentially infinitely ductile in uniaxial compression at ambient pressure, (2) the material containing the low viscosity glass phase can be deformed to nearly 400 percent elongation in uniaxial tension, and (3) with superimposed hydrostatic pressure the material containing the low viscosity glass can be essentially infinitely ductile even in tension.

This discovery suggests that under proper conditions, ceramics with select microstructural features may be sufficiently ductile to permit fabrication of components from them by isothermal forging. This is an important potential forming option since machining of ceramics is both very expensive and has a propensity to produce flaws that lead to unacceptable fracture. Hot-isotatic-pressing, which may be used for near-net-shape forming, has difficulties because large amounts of shrinkage occur during densification making it difficult to produce parts with close tolerances. Metallic superalloys which have been developed for high temperature applications are formed into shape by isothermal forging, but in order to apply the same technology to ceramics it is necessary that ceramics be ductile.

(Cornell University, R. Raj and J-G. Wang)

9. Theoretical Calculations Provide Important Thermodynamic Data for Atmospheric Chemistry Research

With recent advances in computers and theoretical methods the structure and stability of small molecules can be calculated to the best accuracy available from experiment. Such computations can provide thermodynamic data for molecules which are difficult or impossible to study experimentally. These calculations have great potential in the area of environmental chemistry where the thermodynamics of many postulated reactions, which have not been studied experimentally, are necessary to model atmospheric processes, such as acid rain formation. The energetics for the reaction of N_2 with an H atin to form N_2H has been calculated very accurately. The N_2H molecule is a postulated intermediate in acid rain formation as well as in other atmospheric and combustion processes; although, it has not been detected experimentally. A second problem which has been investigated is the energetics for the reaction of CO_2 with H_2O to form $CO_2{:}H_2O$. The $CO_2{:}H_2O$ molecular complex is thought to be involved in the greenhouse effect occurring in the earth's atmosphere, but, again, little is known experimentally about its relative stability and spectroscopic properties.

The calculations on the N_2 + H "reaction surface" indicate that N_2H is probably not an important intermediate in atmospheric or combustion chemistry as had previously been postulated by other workers. The calculations on the CO_2 + H_2O "reaction surface" have provided thermodynamic data for the formation of the $CO_2{:}H_2O$ complex which can be used as input for models being developed to evaluate the greenhouse effect. These data have also provided estimates of the vibrational frequencies of the complex to aid in its spectroscopic detection. These computations illustrate the potential usefulness for *ab initio* "reaction surfaces" in atmospheric chemistry.

(Argonne National Laboratory, L. A. Curtiss and D. L. Drapcho; Carnegie-Mellon University, J. A. Pople; Canisius College, D. Pochatki)

10. New Catalyst Simplifies Direct Conversion of Carbon Monoxide and Water to Methanol

Basic research on homogeneous catalysis, e.g., catalysis induced by catalysts dissolved in solvents, has led to the discovery of a new catalytic system that can promote the direct conversion of carbon monoxide (CO) and water (H_2O) to the fuel, methanol. This conversion can be made to proceed at temperatures and pressures much lower than heretofore necessary for converting CO to methanol. In fact, the yield of methanol is higher with this new catalyst at a pressure of only 10 atmospheres than it is at 100 atmospheres using the present commercial process. Equally or more important is the fact that the new catalytic sequence uses water instead of the far more expensive hydrogen presently required for methanol synthesis. This very promising discovery involves catalysts which are lead compounds dissolved in molten salts. The salts are formed by sodium or similar metals and formic acid. The formate salts and, of course, the lead catalyst are not consumed in the process.

(Argonne National Laboratory, J. W. Rathke & coworkers)

11. Instrumentation Developed for Measurements Underlying Safety and Efficiency of Power Stations

A new method has been developed for in situ, noninstrusive, rapid and nondestructive measurement of the void (bubble) fraction in flowing liquid/bubble systems. It should be especially useful for distinguishing between fundamentally different types of boiling in nuclear and other power reactors, important information for maintaining efficient and safe operation. The concept is based on a sophisticated technique known as Fourier Transform Nuclear Magnetic Resonance, using a nonuniform magnetic field. It allows measuring bubble size, bubble growth (or shrinkage) and bubble velocity, with good dimensional resolultion and with rapid repetition, up to every 36 thousandths of a second. Void densities can be measured for both steady and unsteady flow, with resolution in both time and space. While the method is, so far, limited to one dimensional measurements, it is expected that it will be extended to three dimensions, which would provide widely applicable additional information: bubble shapes and merging or breakup of bubbles.

(University of North Carolina, R. E. Saxe)

12. Increasing the Temperature-Time Series Data Base

The data base for the Northern Hemisphere temperature-time series has been extended back to 1851. Previous data bases began in 1880 to 1900. Additional new records have been obtained worldwide from libraries, archives, and weather data centers. The number of sites for the period 1851 to 1900 was doubled over that of earlier data bases. The improvement in coverage during the late 19th century has resulted in a diminution of the apparent coolness of the period, particularly in the 1880s. The sparse geographic coverage in the original data set for this period resulted in temperature averages that were about 0.1°C lower than the revised values.

On the basis of the extended record, it appears that temperatures remained fairly constant during the second half of the 19th century at close to these levels that prevailed during the 1900s and 1910s, with no temporal fluctuations as have been observed during the 20th century. There is some evidence of a warm period during the first years that records were kept, but this may simply be a result of the restricted spatial coverage during that period. This matter is under investigation, because the occurrence of a period of warmth during the preindustrial period is significant for the detection of CO_2-induced warming.

Data from the 20th century data base are consistent with previous documentations, showing the approximate 0.5°C warming from 1910 to the mid-1940s followed by slight cooling through the early 1970s. A warming trend continued from the early 1970s to the present, with 1981 being the warmest year on record (since 1851) and 1983 being the fourth warmest.

(University of Massachusetts, R. Bradley; University of East Anglia (Norwich, United Kingdom), T. M. L. Wigley)

13. New, Surprising Insight into Combustion Chemistry

The first step in burning hydrocarbon fuels is often the chemical reaction which takes place between an oxygen molecule (two oxygen atoms bound together) and a molecule of the fuel which has lost a hydrogen atom, referred to by chemists as a hydrocarbon radical. But such reactions are hard to study, because the hydrocarbon radicals are hard to prepare in a manageable experimental environment. Recently, ethyl radicals (ethane minus a hydrogen atom) have been prepared with a laser-initiated photochemical method. Their reactions with oxygen molecules have been studied from room temperature up to nearly 1300° C. Experimental results did not support previous assumptions about the chemical mechanisms and rates of these reactions. The expected first step, oxidative breakup of the ethyl radical, does not take place. Instead, the oxygen molecule adds onto the radical, to form a peroxide. The rates of reaction actually decrease as the temperature is raised, so that, at combustion temperatures, the rates are considerably different from those assumed until now by modelers attempting to describe combustion processes. These new experimental results should contribute to improved models, leading to more effective use of present and future fuels.

(Illinois Institute of Technology, D. Gutman)

14. Solid State Electronic Devices for Use at Very High Temperatures

Most transitors in common use quit working when heated above about 200°C. However, progress is being made in building solid-state electronic devices tailored for use at high temperatures. Critical needs for these devices are well-known, for example in reliable instrumentation for jet engine control, geothermal well-logging, and controls for nuclear power plants.

In a major advance, a device called a semiconductor controlled rectifier--a switch--has functioned while red hot, that is at 550°C. This breaks the record for operating temperature for semiconductor devices. This controlled rectifier is a member of a family of devices formed from alloys of gallium, phosphorous, arsenic and aluminum now under intensive study for future energy related applications. Other family members, e.g., transitors and diodes, can also now be expected to function up to 550°C.

This research on instrumentation operable at high temperatures paves the way for widespread advances in measurement methods and process control in hostile environments.

(Sandia National Laboratories-Albuquerque, T. E. Zipperian)

15. Electrochemical Processes Identified as Mechanisms of Wear of Machinery

Until recently it was commonly thought that wear of bearings, gears and other moving machine parts is due mainly to mechanical and chemical causes. Much is known about wear due to abrasive particles, surface imperfections, and corrosion.

In a series of very careful experiments, it has been shown that wear due to electrochemical effects can be about the same as that due to purely mechanical causes. Thus it was found that tool marks or polishing scratches on metal surfaces in contact with one another and moving past each other in a lubricant give rise to localized electric currents much like tiny short-circuited batteries. The accompanying electrolysis wears out the surface at a high rate.

This new knowledge promises new approaches to reducing wear problems in machines. For instance some additives to the lubricant can reduce the electrochemical action and thus lessen damage to the metal surfaces. Results of this research will contribute to increased lifetime of machines used in energy production and utilization.

(Electrochemical Technology Corp., T. R. Beck)

16. Process Design and Control Strategies for Enhanced Energy Efficiency and Productivity Developed

In the past ten years fast changing economic conditions have forced engineers to design process plants which run efficiently not only under some nominal conditions, but also when varying inputs, e.g., price of energy, dictate changes in the way the plant is run.

Recent basic research on adaptive control systems has advanced to the point at which there is taking place a rapid transfer of knowhow from universities to industry. Notable innovations from this research include the first general method for rational synthesis of heat exchanger networks, which is important for better use of process heat in industry. Also, newly found theoretical methods for "resilience" assessment of heat distribution systems have been applied in realistic cases; "resilience" tests the reliability of control systems subject to uncontrollable disturbances. Further, stable use of non-linear controllers has been shown where linear control systems failed to stabilize the system operation.

The results of this pioneering work on process design and control will have a long-term impact on adaptive control research as well as on improving energy use by industry.

(University of Wisconsin, M. Morari, W. H. Ray and D. F. Rudd)

17. New Interpretation of the Volcanic Eruption Process

Combined geophysical techniques and drilling have resulted in several major discoveries this year in the Long Valley caldera region. The Inyo Domes form a line of volcanoes extending northward from the main caldera structure. These volcanoes are the youngest (600 years old) extrusion of the Long Valley magma system. Three DOE drilling projects have penetrated (1) a lava flow at Obsidian Dome volcano, (2) the magma conduit directly under Obsidian Dome, and (3) the deeper dike system that fed magma to the entire Inyo chain. Results to date include: a totally unexpected thermal anomaly persisting in the conduit since the 600 year old eruption; a first-ever direct observation of the 60m diameter conduit consisting of a 30m central channel through which lava flowed freely to the surface and an outer section of fragmented wall-rock intruded by magma; a new interpretation of the eruption process as an extrusion of outgassing silicate foam followed by a cooling period of bubble collapse and welding of glass fragments at the surface to form the currently homogeneous obsidian "lava flow". A full suite of cores and logs were taken in all three holes, and the two deeper holes were successfully cased for future geophysical experiments. Detailed analyses of core and geophysical data are currently under way, but it is already clear that the BES/Geosciences investigations are pioneering an unprecedented scientific understanding of the subsurface anatomy of magma-geothermal systems necessary for the efficient development of their vast energy resources.

(Sandia National Laboratory-Albuquerque, J. C. Eichelberger)

18. Geologic Evidence on the Conditions of Petroleum Formation

Rock samples obtained by drilling into the Green River Shale, an oil producing layer in the Uinta Basin of Utah, has provided direct geological verification of the rate and temperature conditions of petroleum formation. The shale contains kerogen (an organic precursor of petroleum) where it is exposed at the surface on the edge of the Uinta Basin. The same rock layer produces oil from depths of 12,000 to 16,000 feet inside the basin. By combining measurements of the state of compaction of shale samples recovered from drilling to successive depths with data on temperature as a function of depth, investigators were able to reconstruct the time vs. temperature history of the Green River Shale. For the oil producing zone, the average heating rate and maximum temperature achieved during the kerogen to petroleum transition were 5°C increase per million years and 155°C, respectively. This geological reconstruction of the natural conditions of petroleum formation is an excellent agreement with laboratory experiments on the chemical kinetics of converting kerogen to petroleum which indicate a very pronounced maximum in the rate of conversion in the range 150-160°C when the laboratory heating rates (necessarily much faster by many orders of magnitude) are extrapolated back to the natural rate. Because large extrapolations of laboratory data invariably introduce uncertainties about their applicability to natural phenomena, an independent geological confirmation is particularly significant in furthering our understanding of the origin of this fossil fuel.

(Lawrence Livermore National Laboratory, A. K. Burnham)

19. New Free-Electron Laser Amplifier Reaches High Power Levels

Microwave radiation power levels were boosted more than 250,000 percent in a free-electron laser amplifier. A microwave signal was sent through the unique laser amplifier raising the signal's power from 30,000 watts to more than 80 million watts. The amplified signal was measured by three different methods to be certain of its immense power output.

This is the first operation of a free-electron laser as a high-gain microwave amplifier. Previous experiments achieved similar high power microwaves, but they required an additional magnetic field that cannot be used for shorter wavelength radiation.

A free-electron laser amplifier is a device that can transfer energy from a beam of electrons travelling at near light speed (186,000 miles per second) to a beam of electromagnetic radiation, such as microwaves or visible light. The added energy increases the intensity of the electromagnetic beam.

The advantage of a free-electron laser is its efficiency in converting electrical energy into laser light and its ability to be tuned over a wide range of wavelengths. This research offers the additional benefit of being able to produce high-powered pulses of laser light.

Microwaves from a free-electron laser might drastically reduce the length and power requirements of linear accelerators, and could also help confine the fuel in certain types of magnetic fusion reactors.

Most significant to the researchers, however, is their expectation that the demonstration of their high-gain free-electron microwave amplifier will lead to success at shorter wavelengths along the electromagnetic spectrum, including infrared, visible and ultraviolet light, where the amplifier could be used for many laser applications.

(Lawrence Berkeley Laboratory, A. M. Sessler and D. Prosnitz)

20. Large Concentrations of Soot Found in Arctic Air

Large concentrations of soot have been measured at ground-level stations throughout the western Arctic; modeling studies indicated that the soot could lead to heating effects over polar ice. The soot may be responsible for the warming trend indicated by the Arctic temperature-time series which others have attributed to the carbon dioxide (CO_2) buildup.

One of the major uncertainties in modeling the effects of the Arctic haze on the solar radiation balance has been limited knowledge of the vertical distribution of graphitic carbon particles (soot) and their associated solar and infrared absorption coefficients. During 1983 and 1984, the first measurements of such distribution in the Arctic atmosphere were obtained. These measurements were achieved with a new instrument, called an aethalometer, designed at LBL that is capable of determining soot concentrations on a real-time basis.

Part of the data base obtained in 1983 has been analyzed, yielding the following results:

1. Substantial concentrations of soot were found throughout the Arctic atmosphere (i.e., in the Alaskan, Canadian, and Norwegian Arctic areas and the North Pole).

2. Vertical profiles of soot can show either a strongly layered structure or an almost uniform distribution to 8 kilometers (26,000 ft). Concentrations of particles within layers can be as large as those found at ground level in typical midlatitude urban areas.

3. A comparison of the vertical profiles with ground-level measurements indicates that peak concentrations aloft can be significantly greater.

4. The absorption optical depths associated with these vertical profiles are large enough to cause a substantial change in the solar radiation balance over a highly reflective surface such as polar ice.

5. Results of initial modeling studies with the new data have indicated that the soot could be one of the causes of the Arctic warming trends. (Lawrence Berkeley Laboratory, H. Rosen; Lawrence Livermore National Laboratory, M. C. MacCracken)

21. Carbon Dioxide Improves Water-Use Efficiency of Plants

Elevated levels of CO_2 cause increased plant photosynthesis. In addition, stomata (small pores in the leaf through which CO_2 and water vapor are exchanged) partially close in response to increased levels of CO_2, and this decreases plant water loss (transpiration). A concept now being confirmed by new data is that improved water-use efficiency* (WUE) because of elevated levels of CO_2 will measurably increase growth and dry weight gain of plants. This is especially important in situations of low-water availability.

New results of research on the response of plants to CO_2 provide improved quantitative values of photosynthetic WUE for several crops and native species. These results are based on research on whole plants that have been continuously exposed to elevated levels of CO_2 in containment situations that approximate normal field conditions (natural light and temperature). For soybeans and several other species grown inside such containment, it is clear that increased levels of CO_2 cause a doubling of the WUE, and for field-grown corn, the WUE may increase by 35 to 100%.

The accumulating experimental evidence of improved WUE is an important finding for agriculture and ecology because water stress is often regarded as the single most limiting factor for plant growth. Implications of improved WUE include the protection of plants from drought and other stresses, and possibly reduction in the quantity of water required for the plant to complete its life cycle or to produce harvestable yield. Modified WUE could affect water requirements for irrigated croplands and may indirectly affect the distribution of natural plant communities. The possibility has also been proposed that CO_2 may function as a widespread antitranspirant, thereby making water available for other purposes.

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* The conventional expression of the efficiency of water to fix carbon is WUE = carbon fixed/water consumed

(U. S. Dept. of Agriculture; Agronomy Physiology Lab-Gainesville, Florida, H. Allen; Air Pollution Effects Lab - N.C. State, H. Rogers; Crop Simulation Lab - Mississippi State, B. Acock. Lawrence Livermore National Laboratory, J. Shinn)

22. New Theoretical Approach Advances Understanding of Combustion Chemistry

Increased understanding of the combustion process is needed to improve the use of hydrocarbon fuels, increasing the efficiency of their use, and minimizing attendant pollution. A critical aspect of the combustion process requiring detailed understanding is that of extremely rapid chemical reactions. Molecular species exist in, and affect the course of, chemistry in a flame; among these are transient species known as molecular radicals. Their behavior in the flame is strongly affected by internal bond energies. These binding energies between atoms in a molecule are described by the thermodynamic quantity known as heat of formation. This quantity is very difficult, if not impossible, to measure for very short lived transient species. Thus, theoretical calculation of heats of formation is necessary.

Recently, a new theoretical approach has been developed which allows calculation of heats of formation with much greater reliability than before. Using this new approach, it has been shown that previously accepted values for heats of formation of the nitrogen-hydrogen radicals NH and NH_2 are not correct. Further, for the first time, the heats of formation of several other radicals made up of carbon, hydrogen and oxygen atoms have been determined. This new approach will help bring more order and insight to the understanding and exploitation of combustion processes, providing an important new tool for combustion chemists and engineers.

(Sandia National Laboratory-Livermore, Combustion Research Facility, C. Melius and S. Binkley)

23. Balancing the Global Carbon Cycle Improved

A considerable amount of research reported over the past year supports the fact a significant overall lowering of the estimated magnitude of release of both the historical and contemporary amounts of terrestrial carbon. For example, the net amount of carbon released because of contemporary changes in land use has been justifiably revised downward by a significant amount, from a range of 1.8 to 4.7 gigatons of carbon per year to 0.5 to 1.8 gigatons per year (a gigaton, equals 10^{15}g). This has greatly reduced the magnitude of the incompatibility between estimates of oceanic CO_2 uptake and terrestrial CO_2 release. Further, more recent estimates of early atmospheric CO_2 levels based on refined analyses of occluded air in early 19th century ice are 20 parts per million by volume (ppm) higher than values reported previously. The higher values are also more compatible with reduced estimated of terrestrial fluxes.

These new findings continue to suggest that the oceans may be assimilating more CO_2 from the atmosphere than has been estimated until now. Refinements in ocean carbon cycle models averaged for the entire Earth have resulted in estimates of the amount of CO_2 taken up by the oceans that are 25% higher than those established previously. However, current ocean models are still unable to accommodate a significant release of CO_2 from terrestrial ecosystems. Further progress toward balancing the carbon cycle depends on more realistic and geographically detailed models of both the oceanic and terrestrial carbon systems. Development of such models, in turn, depends on an enhanced data base of carbon reservoirs and fluxes in both time and space.

(Oak Ridge National Laboratory, L. Mann; Bern U., Switzerland, Hans Oescher; U. Of Illinois, S. Brown; U. of Puerto Rico, A. Lugo; Marine Biological Laboratory, R. A. Houghton, J. Melillo; Duke U., W. Schlesinger)

24. Photosynthesis Regulation

Photosynthesis, the energy process that provides food, fuel, and fiber for life on earth, is now conceived as having two light driven photosystems that are connected by a biochemical chain called the electron transport system. How the two photosystems are coordinately regulated has been a long standing question. Recent work has produced an explanation for this regulation. The mechanism involves the phosphorylation (adding phosphorous) to some key proteins (light harvesting chlorophyl and protein complex) in response to the oxidation-reduction state of one of the components of the electron transport chain. This mechanism of phosphorylation and de-phosphorylation of photosynthetic proteins affords a more balanced distribution of the trapped light energy between the two photosystems and consequently probably improves the overall efficiency of photosynthesis. The understanding of such control mechanisms is important to designing artificial light trapping devices and could enter into future plant improvement strategies intended to enhance plant (renewable) productivity.

(Brookhaven National Laboratory, J. Bennett)

25. Measurement Made of D-T Reaction to Much Higher Accuracy Than Ever Before

The basic fusion-energy reaction, deuteron + triton leading to alpha + neutron, has been measured to a much higher accuracy than ever before over a range of triton bombarding energies 12.5 to 117 keV, equivalent to plasma temperatures in the kT temperature range from 0.7 to 18.8 keV. This is the operating range of the first generation magnetic- and inertial-confined fusion reactors. The cross section is accurate to 1.4% over most of the energy range, with the error rising to 4.8% at the lowest energy. The measurement featured the use of a windowless, cryogenically pumped gas target, specially designed calorimeters to measure beam current, and special techniques to determine the target gas density. The system will be used to measure the cross sections for the reactions of other hydrogen and helium isotopes at the very low energies of interest to fusion technology and astrophysics.

(Los Alamos National Laboratory, N. Jarmie and R. E. Brown)

26. Increased Beam Intensity for Particle Accelerator Applications

Particle accelerators have been developed for a wide variety of applications, including basic research in high energy physics, nuclear physics, defense, and numerous industrial applications. In spite of decades of increasing both the beam kinetic energy and the beam intensity, the fundamental limits for the transport of intense beams in conventional transport systems have not been well known. Now, as a result of recent research conducted in the Heavy Ion Fusion Accelerator Research (HIFAR) program, these limits have been established. The HIFAR program, initiated to develop and evaluate heavy ion accelerators for inertial fusion energy applications, requires the maximum intensity possible to be successful. The program involves stages of research from single beam experiments to multiple beam accelerator development. A series of single beam experiments have recently been concluded which demonstrate that beam currents three times larger than previously thought possible are now feasible. These results apply not only to the HIFAR program but to a wide variety of other applications.

(Lawrence Berkeley Laboratory, D. Keefe and coworkers)

27. Chemical Purification of Uranium Aids in Isotopic Enrichment

A new concept has been discovered for improved cleanup of uranium hexafluoride (UF_6) gaseous process streams. These streams are central to recovering uranium from partially spent reactor fuel. The cleanup is necessary because certain products of the reactor fuel "burning" contaminate the UF_6 and interfere with the isotope enrichment process for uranium-235. Basic chemical studies found that gaseous metal fluoride impurities in the UF_6, such as neptunium hexafluoride, will react with solid uranium pentafluoride to form solid fluorides of the impurity metals. This removes the impurities from the gas stream. Later, the trapped impurities can be recovered photochemically for theiown value. The applicability of this cleanup procedure for removal of other metal contaminants is being examined.

(Argonne National Laboratory, J. V. Beitz)

28. A New Procedure in Stable Isotope Separation Better Serves Users' Needs

A new approach to operating the calutrons has led to simultaneous separation of isotopes of more than one element within a single magnetic segment. The calutrons are magnetic isotope separators that were built during the World War II Manhattan Project for the enrichment of uranium-235 but which are now used for the enrichment of many other isotopes for use in nuclear medicine, basic research, and industry. The need for a wide variety of isotopes for these applications is now being better met by this new procedure. While this new procedure separates a larger number of elements during a calutron run, it does however result in the production of smaller amounts of each isotope produced per unit of operating time.

(Oak Ridge National Laboratory, E. Newman)

29. Control of Actinide Valence States Important in Nuclear Waste Isolation

Thermodynamic studies have provided important guidelines for using synthetic mineral hosts for nuclear wastes. A candidate procedure for the disposal of the waste materials from the processing of nuclear fuels is to incorporate them into stable solid chemical compounds (hosts) that can be placed for long term storage in a repository. Such a compound could be mixed-metal oxide. To minimize escape of the radioactive wastes from the solid hosts into the ground water, both the hosts and the contained activities must be resistant to chemical degradation and solubility in water. Some of the important waste constituents are heavy actinide elements. It has been found that the plus-six valence state of the actinides is more leachable by water than the plus-four state and therefore the preparation of the solid host material must be carefully adjusted chemically to avoid the more soluble valence state of the actinides.

(Argonne National Laboratory, L. Morss)

30. Theory Challenged: Iron Oxide Clusters Maintain Fe_9O_{10} Ratio

As iron rusts, its atoms pass through more than one state of oxidation. The first of these stages is ferrous oxide, nominally made up of positively charged iron ions (Fe^{++}) and negatively charged oxygen ions (O^{--}) in a one-to-one ratio. But in nature the mineral ferrous oxide is found not to have this one-to-one ratio, having instead only 9 iron ions for every 10 oxygen ions. This has been thought to be due to a chemical action between pairs of iron ions, whereby some of the iron passes out of the mineral. Such behavior is understood in terms of a fully ionic structure, i.e., made up of only positively charged iron atoms and negatively charged oxygen atoms.

Now a new and clever technique has been devised by chemists at Argonne National Laboratory for study of the behavior of metal clusters containing only 2 to 60 metal atoms. Clusters of iron and oxygen atoms in that size range were believed to be unable to exist in a fully ionic structure, and thus unable to interact as described above for pairs of iron ions. The cluster should therefore maintain the one-to-one ratio of iron to oxygen atoms. To everyone's great surprise, what was found in clusters down to a size of 9 iron atoms was the same ratio as in the bulk mineral 9 iron to 10 oxygen atoms. These results demonstrate the need for a whole new approach to understanding the chemical and electronic structure of the iron oxides and, perhaps, of a much wider group of metal oxides. Since ferrous oxide and many other metal oxides are practical or potential semiconductors (transistors, computer chips), these results may lead to further studies having wide ranging benefits.

(Argonne National Laboratory, S. Riley and coworkers)

31. Microbial Population Changes in Anaerobic Digestors

Methanogenesis is a natural process that occurs in many ecosystems where oxygen is at very low levels (anaerobic). Man has harnessed methanogenesis in anaerobic digestors to produce methane gas which is used as a fuel. Despite the widespread occurrence and utilization of methanogenesis, the microbial ecology is still poorly understood. Two recent advances have begun to provide new insights into mechanisms of methanogenesis. During the course of the development of the microbial activity within an anaerobic digestor, it has been observed that the microbial populations change appreciably before stabilization is achieved. These dynamics have now been documented. Also, there has been the development of highly specific immunologic agents produced against various species of methanogenic bacteria which has made identifications easier, faster and more reliable.

With these findings and procedures available it may be expected that a better understanding of anaerobic digestion generally, and methanogenesis specifically, will proceed rapidly. These processes have important environmental implications as well as for the production of fuel, particularly in less developed countries.

(New York State Department of Health, A. J. L. Macario, E. Conway de Macario, and M. J. Wolin, and Cornell U., S. H. Zinder)

32. Electron-Molecule Interactions Important for Excimer Lasers Measured

A scientific breakthrough has been achieved which is important to laser developers. For the first time, absolute measurements have been made of the interaction of electrons with individual molecules which are electrically polar, that is, molecules in which electrons are displaced to produce poles, much like a bar magnet, except that the poles in the molecule are electrical, not magnetic. The previous inability, whether theory or experiment, to provide this kind of information has hampered the understanding and advancement of a class of lasers known as excimer lasers. Previous experimental efforts have been indirect, requiring researchers to rely on theory to interpret their results. But the theory itself has given ambiguous and conflicting results. Now, physicists have cleverly devised an experimental setup for direct measurement of the interaction. The setup involves a beam of cesium bromide vapor intersecting an electron beam. Following the encounters in the intersection of the beams, the emerging molecular ions, molecules and electrons were measured and their energies and angles of emergence determined. The results showed this particular interaction to be one of the longest range ever observed between a point charge and a neutral system (on the scale of molecular dimensions, of course). This achievement was followed up by similar measurements on other polar molecules. The measurements are sure to be used to improve greatly the physical theory of this type of interaction, and should contribute to the practical development of excimer lasers.

(New York University, B. Bederson and B. Jaduszliwer)

33. New Levels of High Static Pressure, 2.5 Mbar, Reached with an Advanced Diamond Anvil Cell

Development of a new design of a diamond anvil pressure cell has resulted in the attainment of a new record static high pressure of 2.5 Mbar (about 38 million psi). The key to the design is the achievement of very precise alignment of the diamond facets, full metal gaskets, and miniaturizing the sample size to about 30 microns in diameter. From initial experiments it appears that pressures as high as 3 Mbar will soon be reached and that the novel technique can be used for a wide class of sample materials, including hydrogen. In these initial experiments on a ruby chip, the ruby fluorescence line - the shift of which is presently used by high pressure scientists as a pressure scale - is lost above 2 - 2.5 Mbar suggesting the ruby itself has become metallic.

The achievement of a static pressure of 2.5 Mbar - almost twice that previously obtained - opens the way for the investigation of materials under extreme conditions and will aid in the search for new materials. An important example is the investigation of hydrogen at multi-Mbar pressures: recent theoretical studies indicate that hydrogen will become metallic at pressures between 3 and 4 Mbar and it is expected to have a very high superconducting transition temperature and a very high Debye temperature (a very hard material). Entirely new classes of materials with unusual and useful properties can be expected to result from research in the very high pressure regime.

(Carnegie Institution, P. Bell and H. K. Mao)

34. New Method for the Analysis of Experimental Nuclear Data

An innovative approach to the treatment of uncertainties associated with experimental data has been developed at ORNL and applied to the analysis of nuclear data. This new technique utilizes group-theoretical methods to treat in a coherent way both statistical and systematic uncertainties.

New approaches developed from this fundamental breakthrough have been implemented in computer programs designed to use well-understood resonance-interaction theory to accurately analyze many thousands of neutron-scattering data points. The complete set of experimental uncertainties, including correlations, is carried through all steps of the analysis, so that the deduced resonance parameters have uncertainties correctly determined from the original experimental uncertainties.

(Oak Ridge National Laboratory, F. G. Perey)

35. The Cosmic Cube, a 64 Processor Computer, is Operational

Researchers have successfully built a 64 processor research computer with the equivalent computing power of one-tenth a Cray-1 at one-hundredth the price. This architecture is dramatically different from today's Class VI machines and early results indicate it may be a cost effective alternative for a variety of scientific problems. The current machine located at California Institute of Technology, uses 64 processors with nearest neighbor or local interconnections amongst processors. It has long been realized that such machines could provide substantial speed up on computations where the interactions amongst objects being computed had a similar local structure; i.e., speed up would be possible if the topology linking the processors mirrored the topology linking the objects being computed. It has been demonstrated that speed ups on such problems were indeed possible, but more importantly, it has now been shown that a large class of problems with non-local interactions could be effectively mapped into ones with approximately local interactions which could then be solved effectively on the Cosmic Cube. A lattice gauge problem modeling fundamental properties of matter ran for 2500 hours on the cube and provided scientists with highly reliable and interesting results on the heavy quark potential. A variety of other problems have been implemented on this machine, including ones from astrophysics, molecular dynamics, geophysics, and critical phenomena in materials.

(California Institute of Technology, G. C. Fox and C. L. Seitz)

36. Capillarity Phenomenon Mathematically Predictable

It has been found that the solution of the equations governing liquid free surface interfaces predicts unexpected behavior if the cross-section of the tube is not circular. It was concluded that the solution of the equations can behave discontinuously or even cease to exist when small changes are made in contact or capillary-tube cross-section. For example, when applied to the case of a wetting liquid in a tube of square cross-section in zero gravity, analysis predicts that for contact angles greater than or equal to a critical value of 45 degrees the height of the free surface (portion of a sphere) is uniformly bounded, but for smaller contact angles no solution of the equation exists. This remarkable behavior was verified experimentally at the NASA-Lewis Research Center in their Zero Gravity Drop Tower. It was observed in tests that for contact angles less than the predicted value the fluid flowed up along the corners rather than remaining simply contained in the bottom of the tube. While these findings have intrinsic mathematical importance, they may find applications in such practical areas as flow in heat pipes, growth of crystals in low gravity, behavior of petroleum in underground reservoirs, and other areas in which capillarity phenomena play a role. The effect of zero-gravity capillarity is important in space manufacturing and will be investigated further in an upcoming space shuttle flight experiment.

(Lawrence Berkeley Laboratory, N. Albright et al; Stanford University, J. Marsden, A. Weinstein)

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Dist. Category UC-25

September 1984

Materials Sciences Programs
Fiscal Year 1984

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences
Washington, D.C. 20545

FOREWORD

The Division of Materials Sciences is located within the Department of Energy in the Office of Basic Energy Sciences. The organizational structure of the Department of Energy is given in an accompanying chart. The Office of Basic Energy Sciences reports to the Director of the DOE Office of Energy Research. The Director of this Office is appointed by the President with Senate consent. The Director advises the Secretary on the physical research program; monitors the Department's R&D programs; advises the Secretary on management of the multipurpose laboratories under the jurisdiction of the Department, excluding laboratories that constitute part of the nuclear weapon complex; and advises the Secretary on basic and applied research activities of the Department.

The Materials Sciences Division constitutes one portion of a wide range of research supported by the DOE Office of Basic Energy Sciences. Other programs are administered by the Office's Chemical Sciences, Biological Energy Research, Engineering and Geosciences, Advanced Energy Projects, and Carbon Dioxide Research Divisions. Materials Sciences research is supported primarily at DOE National Laboratories and Universities. The research covers a spectrum of scientific and engineering areas of interest to the Department of Energy and is conducted generally by personnel trained in the disciplines of Solid State Physics, Metallurgy, Ceramics, Chemistry and Materials Science. The structure of the Division is given in an accompanying chart.

The Materials Sciences Division supports basic research on materials properties and phenomena important to all energy systems. The aim is to provide the necessary base of materials knowledge required to advance the nation's energy programs.

This report contains a listing of research underway in FY 1984 together with a convenient index to the Division's programs. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page. Following that page is a list of the winners of the 1984 Materials Sciences Research Competition, a contest among the major laboratories within the three categories named.

Louis C. Ianniello, Director
Division of Materials Sciences
Office of Basic Energy Sciences

RECENT DIVISION SPONSORED PUBLICATIONS

Topical and Workshop Reports[a]

- High Pressure Science and Technology (1983)
- Scientific Needs of the Technology of Nuclear Waste Containment (1983)
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Radiation Effects (1982)
- Condensed Matter Theory and the Role of Computation (1981)
- Research Opportunities in New Energy-Related Materials (1981)[c]
- Aqueous Corrosion Problems in Energy Systems (1981)[c]
- High Temperature Corrosion in Energy Systems (1981)[c]
- Basic Research Needs and Opportunities on Interfaces in Solar Materials (1981)[c]
- Basic Research Needs on High Temperature Ceramics for Energy Applications (1980)[c]
- Organic Conducting Materials[b]
- Coatings and Surface Modifications[c]
- Novel Methods for Materials Synthesis[b]
- Theory and Computer Simulation of Materials Structures and Imperfections[b]

Summary Research Bulletins (of Work in Progress)[a]

- Ceramic Processing
- Non-Destructive Evaluation
- Sulfur Attack
- Welding

Description of Research Facilities

- Centers for Collaborative Research[a]

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[a] Available in limited quantities from the Division of Materials Sciences.

[b] To be published.

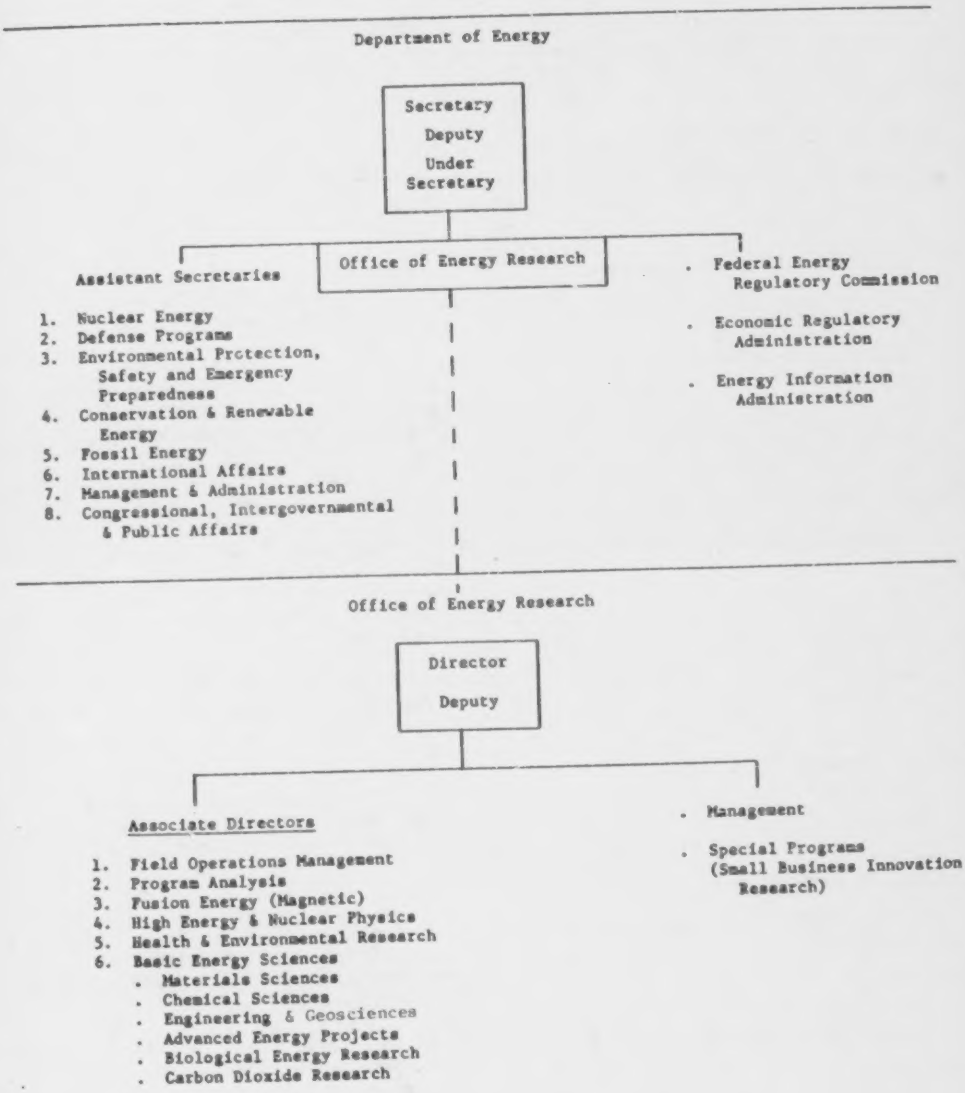
[c] Also published in Materials Science and Engineering.

Winners of the 1984

Materials Sciences Research Competition
Within the DOE Laboratories

Category	Winner(s)
Metallurgy and Ceramics:	
o Outstanding Scientific Accomplishment	H. K. Birnbaum and I. M. Robertson, Univ. of Illinois, "Mechanisms of Hydrogen Embrittlement"
o Sustained Outstanding Research	P. Okamoto, L. Rehn, H. Wiedersich, N. Lam, and R. Averback, ANL, "Radiation-Induced Segregation"
o Significant Implication for Energy Technology	C. T. Liu, C. L. White, and J. A. Horton, ORNL, "Design of Ductile Nickel Aluminides for High Temperature Structural Use"
Solid State Physics:	
o Outstanding Scientific Accomplishment	S. Chiang, P. L. Richards, and R. G. Tobin, LBL, "Infrared Emission Spectroscopy of Chemisorbed Molecules on Metal Surfaces"
o Sustained Outstanding Research	C. P. Slichter, Univ. of Illinois, "Static and Dynamic Properties of Solids"
o Significant Implication for Energy Technology	B. C. Sales and L. A. Boatner, ORNL, "Lead-Iron Phosphate Glass: A New Stable Storage Medium for High-Level Nuclear Waste"
Materials Chemistry:	
o Outstanding Scientific Accomplishment	W. G. Breiland, M. E. Coltrin, and Pauline Ho, SNL-A, "Fundamental Mechanisms of Chemical Vapor Deposition (CVD)"
o Sustained Outstanding Research	M. Blander, ANL, "Application of Thermodynamics to Materials Science"
o Significant Implication for Energy Technology	A. R. Krauss, ANL, "Self-Sustaining, Low-Z Coatings for Magnetic Confinement Fusion Applications"

ORGANIZATION OF THE DEPARTMENT OF ENERGY



Department of Energy

Secretary
Deputy
Under Secretary

Office of Energy Research

Assistant Secretaries

1. Nuclear Energy
2. Defense Programs
3. Environmental Protection, Safety and Emergency Preparedness
4. Conservation & Renewable Energy
5. Fossil Energy
6. International Affairs
7. Management & Administration
8. Congressional, Intergovernmental & Public Affairs

- Federal Energy Regulatory Commission
- Economic Regulatory Administration
- Energy Information Administration

Office of Energy Research

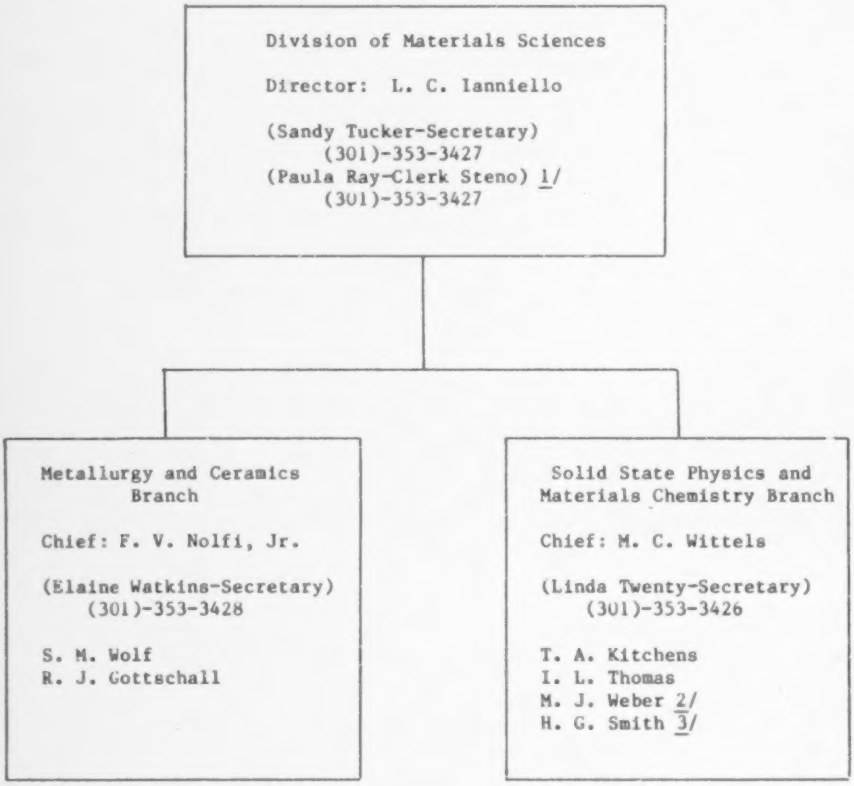
Director
Deputy

Associate Directors

1. Field Operations Management
2. Program Analysis
3. Fusion Energy (Magnetic)
4. High Energy & Nuclear Physics
5. Health & Environmental Research
6. Basic Energy Sciences
   - Materials Sciences
   - Chemical Sciences
   - Engineering & Geosciences
   - Advanced Energy Projects
   - Biological Energy Research
   - Carbon Dioxide Research

- Management
- Special Programs (Small Business Innovation Research)

OFFICE OF BASIC ENERGY SCIENCES, Division of Materials Sciences Structure



Division of Materials Sciences

Director: L. C. Ianniello

(Sandy Tucker-Secretary)
(301)-353-3427
(Paula Ray-Clerk Steno) 1/
(301)-353-3427

Metallurgy and Ceramics Branch

Chief: F. V. Nolfi, Jr.

(Elaine Watkins-Secretary)
(301)-353-3428

S. M. Wolf
R. J. Gottschall

Solid State Physics and Materials Chemistry Branch

Chief: M. C. Wittels

(Linda Twenty-Secretary)
(301)-353-3426

T. A. Kitchens
I. L. Thomas
M. J. Weber 2/
H. G. Smith 3/

Notes: 1/ Temporary Assignment from Energy Research Administrative Office
2/ On Leave from Lawrence Livermore National Laboratory
3/ On Leave from Oak Ridge National Laboratory

INTRODUCTION

The purpose of this report is to provide a convenient compilation and index of the DOE Materials Sciences Division programs. This compilation is primarily intended for use by administrators, managers, and scientists to help coordinate research.

The report is divided into six sections. Section A contains all Laboratory projects, Section B has all contract research projects, Section C has projects funded under the Small Business Innovation Research Program, Section D has information on DOE collaborative research centers, Section E gives distributions of funding, and Section F has various indexes.

Each project in Sections A, B, and C carries a number (at the left hand margin) for reference purposes, e.g., in Section F. The FY 1984 funding level, title, personnel, budget activity number (e.g., 01-2) and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), or Materials Chemistry (03). The budget numbers carry the following titles:

01-1 - Structure of Materials
01-2 - Mechanical Properties
01-3 - Physical Properties
01-4 - Radiation Effects
01-5 - Engineering Materials

02-1 - Neutron Scattering
02-2 - Experimental Research
02-3 - Theoretical Research
02-4 - Particle-Solid Interactions
02-5 - Engineering Physics

03-1 - Chemical Structure
03-2 - Engineering Chemistry
03-3 - High Temperature and Surface Chemistry

Section D contains information on special DOE centers that are operated for collaborative research with outside participation. Section E summarizes the total funding level in a number of selected categories. Most projects have been classified under more than one category since the categories are not mutually exclusive. In Section F the references are to the project numbers appearing in Sections A, B, and C and are grouped by (1) investigators, (2) materials, (3) techniques, (4) phenomena, and (5) environment.

It is impossible to include in this report all the technical data available for the program in the succinct form of this Summary. To obtain more detailed information about a given research project, please contact directly the investigators listed.

Preparation of this FY 1984 summary report was coordinated by T. A. Kitchens. Though the effort required time by every member of the Division, most of the work was done by Miss P. Kay and Mrs. L. Twenty, who also kept the effort on track. This year the Summary was done "by the computer." This could not have been accomplished without the very competent professional assistance of Mrs. K. Roskin, Calculon, Inc.

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SECTION A

Laboratories

The information in this section was provided by the Laboratories. Most projects are of a continuing nature although specific projects were concluded and others initiated this fiscal year.

LABORATORIES

AMES LABORATORY
Iowa State University
Ames, Iowa 50011

Metallurgy and Ceramics - 01 -

D. T. Peterson - Phone (FTS) 865-4446 or 515-294-4446

001. MATERIALS SCIENCE OF INTERFACES

A. J. Bevolo, F. C. Laabs, L. M. Seaverson
Phone: (515)-294-5414
$202,000 01-1

Studies of interface structure and composition using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Core level and plasmon spectra of pure rare earth metals using ELS and Auger. Auger spectroscopy of metallic hydrides for phase identification. Effects of tin alloying on brass corrosion behavior in aqueous salt solutions. Scanning Auger microprobe analysis (35nm) of grain boundary inclusions in carbonized low alloy steels and effects of radiation on the competition between C and P grain boundary segregation in iron. Local chemical state information from Auger lineshape analysis in Fe-B-Be metallic glasses.

002. NONEQUILIBRIUM MATERIALS

S. J. Poon, A. J. Drehman, A. R. Pelton
Phone: (515)-294-4736
$255,000 01-1

Studies of metallic glasses, metastable crystalline phases and extremely fine microstructural alloys. Ultra high vacuum melt spinning apparatus to process reactive metals without contamination. Directional solidification apparatus modified to achieve extremely large undercooling and solidification rates. High speed planar solidification of eutectic Pd-Cd. Microstructural study by TEM of transformation products of decomposition of metallic glasses and of rapidly crystallized solids.

003. SURFACES AND SOLIDIFICATION

R. K. Trivedi, J. T. Mason
Phone: (515)-294-5869
$206,000 01-1

Theoretical and experimental studies of the effect of temperature gradient, growth rate and composition on the stability and steady-state shape of solid-liquid interfaces obtained during controlled solidification. Study of morphological transition from dendritic to cellular to eutectic structure. Experimental work on primary dendrite spacing, eutectic spacing and interface structures in Pb-Sn, Pb-Au, Pb-Pd and Pb-Bi systems. Study of interface stability and morphological characteristics in model transparent materials such as succinonitrile and acetone mixtures. Microstructure development during amorphous to crystalline transition.

LABORATORIES

AMES LABORATORY (continued)

004. MICROSTRUCTURAL CONTROL IN METALS

J. D. Verhoeven, E. D. Gibson
Phone: (515)-294-9471
$297,000 01-1

Production of Nb_3Sn-Cu and V_3Ga-Cu superconducting wire by the in situ process, study of problems on the addition of Sn and Ga by the external diffusion method and evaluation of filament cross linking within the microstructure. A study of directionally transformed pearlite versus applied stress level and temperature gradient. The mechanical properties of in situ prepared Cu-base composite alloys. Directional solidification studies on segregation and morphology in grey, nodular and white cast iron. Evaluation of microstructural changes in the austempering of nodular cast irons. Microstructure evolution under solidification conditions typical of welding processes.

005. MECHANICAL METALLURGY

W. A. Spitzig, J. Kameda, J. Kasichainula
Phone: (515)-294-5082
$400,000 01-2

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Hydrogen diffusion in vanadium base alloys by internal friction. Hydrogen induced brittle cracking in low hydrogen solubility bcc metals and alloys. Studies on the effects of radiation-induced defects and solute segregation on intergranular embrittlement. Modeling of hydrogen embrittlement. Description of three dimensional arrays of defects and relationship of arrangement to ductility and mechanical properties.

006. STRUCTURE AND PROPERTY RELATIONS IN METALS

J. F. Smith
Phone: (515)-294-5083
$86,000 01-3

Development of thermodynamic functions for alloy formation in Y-Fe, Y-Co, and Y-Ni systems from electromotive force measurements to test the conflicting predictions of the Bennett-Watson theory and the Miedema theory. Computer analysis of thermodynamic data for the prediction of stable and metastable phase equilibria, metallic glass formation, and control of microstructures.

LABORATORIES

AMES LABORATORY (continued)

007. TRANSPORT STUDIES

O. N. Carlson
Phone: (515)-294-2375
$190,000 01-3

Study of fast diffusion and electrotransport of metallic solutes in scandium and thorium. Measurement of transport parameters for iron, in scandium and cobalt thorium as a function of temperature and determination of activation energies for diffusion. Investigation of mechanism and type of defect responsible for fast diffusion of cobalt in thorium by use of internal friction and scanning electron microscopy. Thermotransport of interstitial solutes in vanadium-titanium alloys. Mass transport of carbon in two-phase Nb-C and V-C alloys in presence of temperature gradient. Precise determination of solid solubility of carbon in vanadium.

008. HYDROGEN IN METALLIC SOLIDS

D. T. Peterson
Phone: (515)-294-6585
$257,000 01-3

Diffusion, thermotransport, and solubility of H and D in V alloys with Ti, Cr, Al or O. Photoelectron spectroscopy, and metallography of metal hydrides and solid solutions of H in vanadium base alloys. Local mode energies for hydrogen in metals and metallic solids.

009. RARE EARTH MATERIALS

K. A. Gschneidner Jr., S. K. Dhar, P. Manfrinetti
Phone: (515)-294-2272
$252,000 01-3

The influence of composition and impurities on the quenching of spin fluctuations and other magnetic phenomena in: (1) highly enhanced paramagnets RCo_2 (R=Sc, Y and Lu), Sc and Pd-Ni alloys; (2) valence fluctuation materials $CeSn_x$ ($x \simeq 3$) and $CeSi_x$ ($x \simeq 1.8$) alloys; and (3) itinerant ferromagnets Sc_3In and $ZrZn_2$. Low temperature (1-20 K) - high magnetic field (1-10 T) heat capacity, magnetic susceptibility (1-300 K, 0.9 to 1.5 T), resistance ratio ($\rho_{300}/\rho_{4.2}$), metallography and lattice parameters measurements are being used to characterize the various behaviors. Nonequilibrium phases resulting from solidification and phase transformations in rare earth based alloys.

LABORATORIES

AMES LABORATORY (continued)

010. NDE MEASUREMENT TECHNIQUES

O. Buck, R. B. Thompson, C. V. Owen, D. K. Rehbein, D. C. Jiles, J.-M. Baik
Phone: (515)-294-3930
$383,000 01-5

Techniques to measure failure related material properties are investigated. Dual objectives of improving understanding of failure mechanisms and inspection reliability. Ultrasonic measurement of internal stresses. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide detailed information about closure condition near crack tip and to determine the influence of this condition on detectability. Microscopic characterization and modeling of the effects of stress and deformation on crack initiation and growth of brass under corrosive conditions. Relationship between fatigue damage or stress on magnetic properties.

011. PROCESSING OF CERAMICS

M. Akinc, G. W. Jordan, M. D. Rasmussen
Phone: (515)-294-6964
$252,000 01-5

Effect of processing variables on characteristics of ceramic powders. Influence of hydroxide precursor dewatering treatments on morphology, surface characteristics, compaction and sintering behavior of oxide powders produced from them.

012. ADVANCED MATERIALS AND PROCESSES (see also page D-25)

F. A. Schmidt, O. D. McMasters
Phone: (515)-294-5236 or (515)-294-1562
$170,000 01-5

Processing of refractory and strategic metals. New process for preparing kilogram quantities of high purity vanadium. Development of arc melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys containing uniform dispersion of the refractory metal. Processing of stoichiometric and non-stoichiometric materials by an inductively coupled plasma. Measurement of diffusion and electrotransport behavior of solutes in rare-earth and refractory metals and the application of these parameters for maximum purification of the host metals. Processing of single crystals of pure metals, solid solution alloys, and intermetallic compounds, both congruent melting and peritectic in nature, by levitation zone melting in cold crucible, free standing vertical zone melting, Bridgman, Czochralski and strain-anneal recrystallization. Above research being conducted in the Materials Preparation Center described in the Section-Collaborative Research Centers.

AMES LABORATORY (continued)

Solid State Physics Division - 02 -

B. N. Harmon - Phone (FTS) 865-7712 or 515-294-7712

013. NEUTRON SCATTERING

W. A. Kamitakahara, J. Mizuki, C. Stassis, J. Zarestky
Phone: (FTS) 865-4224 or (515)-294-4224
$360,000 02-1

Study of the lattice dynamics, thermodynamic properties, and structural transformations of metals at high temperatures (bcc and fcc La); structure and diffusion in metal hydrides (ScH_x, LaH_x); dynamics and phase transitions of alkali-graphite intercalation compounds; electronic structure and phonon spectra of mixed valence compounds ($CePd_3$, α-Ce, $YbAl_2$); relation of electron-phonon interaction to superconductivity (La, $LaSn_3$). High pressure studies (α-Ce, La).

014. SEMICONDUCTOR PHYSICS

H. R. Shanks
Phone: (FTS) 865-6816 or (515)-294-6816
$200,000 02-2

Preparation and characterization of thin films, rf sputter desposition of amorphous semiconductors including aSi, aSi-C, aGe, aGe-C and AlN, ionized cluster beam and deposition of Si, heteroepitaxy on compound substrates, surface and interface characterization with LEED, Auger, LEELS, photodeflection and IR absorption spectroscopy, measurements of gap state densities using DLTS, SCLC, and C-V on Schottky barriers.

015. SUPERCONDUCTIVITY

D. K. Finnemore, J. R. Ostenson, E. L. Wolf, T. P. Chen, Y. Q. Zhou
Phone: (FTS) 865-3455 or (515)-294-3455
$430,000 02-2

Electron tunneling spectroscopy and surface physics studies of strong coupled transition metal superconductors, including alloys and compounds. Conventional and proximity electron tunneling spectroscopy (PETS) of the electron-phonon spectrum $\alpha^2F(\omega)$. Auger electron spectroscopy (AES), electron energy loss spectroscopy (ELS) and ultraviolet photoemission spectroscopy (UPS). Fundamental studies of superconductivity in inhomogeneous materials; use of Josephson junctions to study flux pinning of isolated vortices, development of materials with very low pinning, and studies of the motion quantized vortices in SNS junctions; development of superconducting composites suitable for large scale magnets in the 8 to 16 Tesla range; practical studies to improve wire fabrication techniques; development of magnetic shielding devices.

LABORATORIES

AMES LABORATORY (continued)

016. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS

D. W. Lynch, C. G. Olson, D. M. Wieliczka
Phone: (FTS) 865-3476 or (515)-294-3476
$290,000 02-2

Electron photoemission and optical properties (transmission, reflection, ellipsometry, electroreflectance) of solids in the visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation Ce and Ce-compounds (e.g., $CeSn_3$), Fe-based alloys with Si and Al, amorphous SiC, benzotriazol on Cu; electroreflectance of emersed Ag electrodes, photon- and electron-stimulated desorption of neutral atoms from insulators.

017. NEW MATERIALS AND PHASES

R. N. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson,
P. Klavins, D. R. Torgeson
Phone: (FTS) 865-5435 or (515)-294-5435
$520,000 02-2

Synthesis and characterization of new ternary compounds such as Chevrel phases, ternary transition metal borides and rare-earth transition metal silicides and phosphides. Study of the physical properties of these new materials, such as microhardness, phase equilibria and their refractory nature, and high temperature behavior. Properties of new ternary phases at low temperatures, including magnetic susceptibility, transport properties, heat capacity, crystallographic phase transformations, coexistence of superconductivity and long range magnetic order. High pressure equations of state of new materials, elementary solids (alkali and alkaline earth metals); effects of hardness on thermal expansivities of technical materials (beryllium copper); low temperature expansivity of materials (Lu) containing hydrogen. Applications of NMR to hydrogen embrittlement of refractory metals (V, Nb, Ta) and alloys (V-Ti, Nb-V), trapping of hydrogen by interstitial impurities in these metals, structural and electronic characterization of hydrogenated amorphous Si, Ge, SiC, and GeC films.

AMES LABORATORY (continued)

018. MATERIALS FOR HYDROGEN STORAGE

R. G. Barnes, J. D. Corbett, K. A. Gschneidner Jr.,
W. A. Kamitakahara, D. T. Peterson
Phone: (FTS) 865-4754 or (515)-294-4754; (515)-294-1560
$185,000 02-2

Interdisciplinary study of metal-hydrogen interactions for development of better hydrogen-storing materials. Materials studied include hydrides of transition metals (e.g., YH_2), refractory alloys (e.g., V-Ti-H), rare-earth-transition metal compounds (e.g., $Y(Al,Ni)_5$-H), and low-valent and lower-dimensional compounds of Group III and IV metals (e.g., LaCl-H, ZrCl-H). Properties and methods include hydrogen locations, super structures, phase transformation, electronic density-of-states, hydriding kinetics, enthalpies of hydride formation, hydrogen diffusion, low-temperature heat capacity, X-ray and neutron diffraction, nuclear magnetic resonance, XPS and UPS.

019. X-RAY DIFFRACTION PHYSICS

J.-L. Staudenmann, D. S. Robinson
Phone: (FTS) 865-3585 or (515)-294-3585 (office);
(515)-294-9614 (laboratory)
$235,000 02-2

X-ray diffraction studies of semiconducting compounds, epitaxial layers, and superlattices. X-ray studies of La at high pressures. Electron charge density studies of V_3Si and Fe-Ni-C in the vicinity of the martensitic phase transition. MATRIX PRT beam line at NSLS.

020. ELECTRONIC AND MAGNETIC PROPERTIES

B. N. Harmon, K.-M. Ho, M. Luban, D. Misemer, M. Nolan, J. Zhu
Phone: (FTS) 865-7712 or (515)-294-7712
$410,000 02-3

Theory of phonon anomalies, lattice instabilities and soft modes in metals and their relation to the electron-phonon interaction and superconductivity (Nb, Mo, Zr, Ti). Total energy frozen phonon calculations for high temperature bcc to ω-phase transition and lattice dynamics. Surface electronic structure of metal electrodes (e.g., Ag), electroreflectance, and microscopic properties of the metal-electrolyte interface. Static and dynamic properties of mixed valence compounds ($CeSn_3$). Electronic properties and chemical bonding of transition and rare-earth metal compounds (ZrB_2, $ZrSe_3$, ZrS, TiS, PtTe, LaH_2, LaH_3, ScH_2). Vacancy formation and ordering (Sc_xS). Renormalization group studies of phase transitions. Electron localization in disordered metals.

AMES LABORATORY (continued)

021. OPTICAL AND SURFACE PHYSICS THEORY

R. Fuchs, K.-M. Ho, S. Auluck
Phone: (FTS) 865-3675 or (515)-294-3675
$160,000 02-3

Optical properties of metals, semiconductors, and insulators; studies of surfaces, thin films, layered systems, small particles, and powders. Differential surface reflectance spectroscopy. Raman scattering from molecules adsorbed on metal surfaces. Surface electronic structure of metal electrodes (e.g., Ag), electroreflectance, and microscopic properties of the metal-electrolyte interface. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrosion effects; anodic photocurrents; the liquid-metal interface. First principles calculation of lattice relaxation and reconstruction at single crystal surfaces (Al, Au).

022. SUPERCONDUCTIVITY THEORY

J. R. Clem, V. G. Kogan
Phone: (FTS) 865-4223 or (515)-294-4223
$120,000 02-3

Electrodynamics of superconductor-normal metal composites; properties of current-carrying type-I and type-II superconductors containing magnetic flux; induced voltages and energy dissipation due to flux motion; vortex nucleation and surface pinning; flux-line cutting in arrays of nonparallel vortices; critical currents and flux pinning in inhomogeneous superconductors; ac losses; two-dimensional Josephson junction arrays; superconducting magnetic shielding.

LABORATORIES

AMES LABORATORY (continued)

Materials Chemistry Division - 03 -

L. E. Burkhart - Phone (FTS) 865-8074 or 515-294-8074

023. X-RAY AND NEUTRON CRYSTALLOGRAPHY

R. A. Jacobson, B. J. Helland
Phone: (515)-294-8444
$185,000 03-1

Determination of atomic arrangements in crystalline and non-crystalline materials by x-ray and neutron diffraction, and EXAFS spectroscopy. Development of diffraction techniques for single crystal and non-single crystal specimens, techniques for pulsed-neutron and synchrotron radiation facilities, and use of Patterson superposition methods. Atom-atom pair correlation functions for non-crystalline materials. Materials studied include rare-earth superconductors, model homogeneous catalysts, polymetal species, complex molybdates, and sulfides, and other substances where intramolecular solid state interactions can modify properties of the parent species.

024. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS

J. D. Corbett
Phone: (515)-294-3086
$175,000 03-1

Synthesis, structure and bonding in intermetallic systems - new Zintl phases, new ternary compounds showing bonding of the type found in A15 phases, interstitials. Reactions and stabilities of phases in the system $CsI-Zr-ZrI_2-ZrO_2$, effects of common impurities, the fate of the important fission products. Low temperature routes to rare-earth oxychlorides and their application to oxygen removal from metals. Properties of metal structures stabilized by interstitial nonmetals including hydrogen. Techniques include high temperature reactions, phase equilibria, transport and crystal growth in inert metal containers, X-ray diffraction, bonding studies by photoelectron spectroscopy, extended Huckel calculations.

LABORATORIES

AMES LABORATORY (continued)

025. CHEMISTRY OF HEAVY TRANSITION METALS

R. E. McCarley
Phone: (515)-294-8680

$170,000 03-1

Synthesis, structure and properties of new ternary oxide phases containing heavy transition elements, especially reduced compounds with metal-metal bonded structures stable at high temperatures. Study of new oxide materials having low dimensional electrical properties, framework, or layer structures which promote high cation mobility for ion-exchange and ionic conductivity, and one-dimensional growth for high strength fibrous ceramics. Correlation of structure and bonding with d-electron count, and relations between structure and physical properties. Experimental methods include X-ray diffraction, photoelectron spectroscopy, resistivity measurements, tensile strength measurements, Mossbauer spectroscopy, and nuclear magnetic resonance.

026. PARTICULATE PROCESSING

L. E. Burkhart, A. Cahill
Phone: (515)-294-8074

$305,000 03-2

Preparation and characterization of ceramic powders with emphasis on liquid-phase methods. Control of nucleation, growth, agglomeration, and morphology to produce powders that sinter to high densities. Quantitative characterization of agglomerates (mechanisms, strength distributions) and correlation with sintering behavior. Theoretical studies include DLVO theory for particle-particle interactions, coagulation and population balance equations for agglomeration kinetics, and Fourier and fractal analysis for morphology. Experimental techniques used are SEM-TEM microscopy, BET surface areas, X-ray diffraction, mercury porosimetry, and image analysis.

027. CARBOTHERMAL PROCESSING OF NON-OXIDE CERAMICS

G. Burnet, M. J. Murtha
Phone: (515)-294-5840

$185,000 03-2

Investigation of reaction mechanisms and kinetics of the preparation of ceramic powders by carbothermal processing, with emphasis on silicon nitride and silicon nitride-based materials. Experimental methods include the use of direct-coupled electrobalance and gas chromatography systems.

LABORATORIES

AMES LABORATORY (continued)

028. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS

H. F. Franzen
Phone: (515)-294-5773

	$255,000	03-3

Study of refractory and corrosion-resistant materials such as transition metal aluminides (Zr-Al, Ta-Al), phosphides and sulfides by both experimental and theoretical techniques to understand the relationships among crystal structure, chemical bonding, and electronic structure as they affect high temperature stability, phase equilibria, and order-disorder transitions. Experimental methods include X-ray and electron diffraction for structure analysis, computer automated simultaneous mass loss-mass spectrometry for high temperature vaporization reactions related to stability, and photoelectron spectroscopy for the electronic structure of solids. Electronic structure studies also include a program of band structure calculations.

029. SURFACE CHEMISTRY AND CATALYSIS

R. S. Hansen, K. G. Baikerikar, D. C. Johnson, P. A. Thiel
Phone: (515)-294-2770

	$335,000	03-3

Evaluation of mechanisms of catalytic reactions, especially hydrogenation, hydrogenolysis, methanation, and hydrodesulfurization reactions, by surface characterization and kinetic techniques, with emphasis on single crystal and evaporated film catalysts. Variation of surface intermediates with surface morphology and of surface reactivity with surface structure. Chemistry of electrode reactions, including electrocatalysis and corrosion reactions. Characterization of electrocatalytic materials by modulated hydrodynamic voltammetry. Reactivity of oxidized and doped electrode surfaces, including characterization of oxygen mobility and defect density at such electrodes. Surface chemistry of nucleation and flocculation applied to ceramic processing. Techniques used include low energy electron diffraction, Auger and scanning Auger electron spectroscopy, infra-red emission and electron energy loss spectroscopies, ring-disk and modulated hydrodynamic voltammetry.

LABORATORIES

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science and Technology Division

F. Y. Fradin - Phone (FTS) 972-4925 or 312-972-4925
H. Wiedersich (01) - Phone (FTS) 972-5079 or 312-972-5079
M. B. Brodsky (02) - Phone (FTS) 972-5016 or 312-972-5016
D. M. Gruen (03) - Phone (FTS) 972-3513 or 312-972-3513

Intense Pulsed Neutron Source Program

G. H. Lander - Phone (FTS) 972-5518 or 312-972-5518

040. DEFECTS IN METALS

R. W. Siegel, R. Benedek, M. J. Fluss, N. Q. Lam, J. N. Mundy,
J. E. Robinson, L. C. Smedskjaer, D. G. Westlake, R. Prasad
Phone: (312)-972-4963
$1,408,000 01-3

Research on the nature and physical properties of intrinsic and extrinsic atomic defects and their interactions in metals and alloys, and the relationship between these and the atomic mechanisms of diffusion under equilibrium and non-equilibrium conditions and the properties of metallic materials; investigations of atomic and defect diffusivities; equilibrium defect formation and concentrations; interactions of atomic defects with one another, with solute atoms, and with interfaces and surfaces; hydrogen interactions with metallic systems; studies of metals (with emphasis on refractory bcc metals), alloys, intermetallic compounds, and amorphous metallic systems with experimental techniques such as positron annihilation spectroscopy, radio-tracer diffusion, resistometry, perturbed angular correlation, transmission and scanning electron microscopy, neutron and x-ray diffraction, and ion-scattering spectroscopy, and the complementary theoretical methods of molecular statics and dynamics, computer modeling, and electronic structure calculations.

041. DEFECTS IN CERAMICS

N. L. Peterson, K. L. Merkle, G. E. Murch, J. L. Routbort, D. Wolf, K. Hoshino, M. P. Thomas
Phone: (312)-972-4955
$848,000 01-3

Diffusion mechanisms and point-defect studies in metal oxides as a function of oxygen partial pressure at high temperatures using cation and oxygen tracer diffusion, conductivity and TEM techniques; impurity diffusion mechanisms, defect-solute interactions and defect clustering in oxides; computer modeling of diffusion processes at dislocations and in non-stoichiometric compounds; TEM studies of dislocation structures in grain boundaries in oxides; theory of defect kinetics, vibration entropy, and atomic structure in grain boundaries; grain boundary diffusion in metal oxides; diffusion mechanisms and impurity interactions in mixed-alkali silicate, alkali borate, alkali germanate, alkali-germanium-sulfur, and alkali-silicon-sulfur glasses; effect of nonstoichiometry and defect clusters on mechanical deformation of oxides; preparation of single and bicrystals of metal oxides.

042. NEUTRON IRRADIATION STUDIES

M. A. Kirk, R. C. Birtcher, B. A. Loomis
Phone: (312)-972-4998
$434,000 01-4

Fast neutron irradiation effects in solids studied using the Radiation Effects Facility at IPNS and in-situ ion irradiation in the HVEM facility; structure and properties of cascades, interactions of free interstitials and vacancies and their clusters in metals and alloys using resistivity, ordered alloys, TEM, and electron irradiation probe techniques; interactions of gliding dislocations with neutron irradiation produced defect structures studied in the HVEM in niobium, vanadium and their alloys; the collapse of defect cascades to dislocation loops studied in the HVEM in Cu_3Au and Fe following low temperature in-situ ion irradiatons; low temperature defect production and annealing in semiconductors studied with resistivity and deep level transient spectroscopy; superconducting property changes in various metallurgical states of Nb-Ti following fast neutron irradiation at 5K; changes in mechanical properties of organic composite insulators following fast neutron irradiations at 5 and 300 K.

LABORATORIES

ARGONNE NATIONAL LABORATORY (continued)

043. IRRADIATION AND KINETIC EFFECTS

L. E. Rehn, R. S. Averback, S. Majumdar, P. R. Okamoto,
R. B. Schwarz, N. J. Zaluzec, J. Don, J. Mansfield, D. Peak
Phone: (312)-972-5021
$1,135,000 01-4

Investigations of mechanisms leading to the formation of defect aggregates, precipitates and other inhomogeneous distributions of atoms in solids with and without displacement-producing irradiation; surface layer modification of alloys by ion implantation, ion-beam mixing, and sputtering; radiation-induced segregation to internal and external defect sinks; effects of irradiation on alloy composition and microstructure; in-situ studies of ion and electron bombardment in the High Voltage Electron Microscope; mechanistic studies of deformation and mechanical strengthening in alloys; ion-beam analysis, analytical electron microscopy; radiation sources include HVEM-2MV Tandem facility and two 300 kV ion accelerators.

044. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH (see also page D-15)

A. Taylor, R. W. Siegel, N. J. Zaluzec
Phone: (312)-972-5109
$666,000 01-4

Development and use of high-voltage and high-resolution analytical microscopy for materials research; operation and development of the Center's 1.2 MeV High Voltage Electron Microscope-Tandem Facility with in-situ capability for direct observation of ion-solid interactions and ion-beam analysis; the HVEM is currently being utilized for research programs in advanced materials, mechanical properties, irradiation effects, oxidation and hydrogenation effects; HVEM specimen stages are available for heating (1300 K), cooling (10 K), straining, and gaseous environments; ion-beam interface with 300 kV ion accelerator and 2 MV tandem accelerator available for in-situ implantations and irradiations; approximately 50% of HVEM usage is by non-ANL scientists on research proposals approved by the Steering Committee for the Center that meets every six months. A state-of-the-art, medium-voltage, ultra-high vacuum Analytical Electron Microscope is being acquired; its design is directed toward the attainment of the highest microanalytical resolution and sensitivity; fundamental studies of electron-solid interactions and microcharacterization of materials, using TEM, STEM, XEDS, and EELS, are conducted at present on lower-voltage (120 kV) instruments.

ARGONNE NATIONAL LABORATORY (continued)

045. OXIDATION STUDIES

N. L. Peterson, W. E. King, K. Natesan, D. J. Baxter,
S. J. Rothman, K. Hoshino
Phone: (312)-972-4955
$658,000 01-5

Point defects and diffusion mechanisms in protective-oxide scales; grain-boundary diffusion in pure and doped protective-oxide materials; studies of adhesion and morphology of oxide scales on crystalline and amorphous alloys using analytical-electron-microscopy techniques; mechanisms and kinetics of oxide film breakdown in bioxidant atmospheres.

046. AMORPHOUS METALLIC ALLOYS

R. B. Schwarz, T. I. Morrison, D. G. Westlake
Phone: (312)-972-4979
$150,000 01-5

Investigations of the synthesis of amorphous metallic materials by isothermal solid-state reactions at the interfaces of vacuum-deposited pure metallic films and mechanically alloyed powders, and by hydrogenation/dehydrogenation reactions; X-ray diffraction, electron microscopy, and Rutherford backscattering studies of the morphology and kinetics of the crystalline-to-amorphous transformation; investigations of the relationships between the atomic structure of amorphous alloys and their magnetic, mechanical and corrosion properties; consolidation of amorphous powders by hot pressing and dynamic compaction.

047. NEUTRON AND X-RAY SCATTERING

D. L. Price, T. O. Brun, J. E. Epperson, J. Faber, G. P. Felcher,
J. D. Jorgensen, P. R. Roach, M. Arai, R. O. Hilleke, C. K. Saw,
M. H. Mueller
Phone: (312)-972-5475
$1,465,000 02-1

Exploitation of neutron and X-ray scattering techniques in the study of the properties of condensed matter. Instrument development and interactions with university and industrial users at IPNS-I and NSLS. Investigations of the structure and defects of ternary superconductors; chalcogenide, oxide, and silicate glasses; surface magnetism; alloy mixing produced by neutron irradiation; residual stresses in deformed materials; decomposition of binary alloys; nuclear magnetic ordering; excited states of hydrogen in metals; magnetism in rare-earth noble-metal compounds; atomic momentum distributions with deep inelastic scattering; mixed conducting lithium electrodes.

ARGONNE NATIONAL LABORATORY (continued)

048. CHEMICAL AND ELECTRONIC STRUCTURE

J. M. Williams, M. A. Beno, C. D. Carlson, A. J. Schultz,
R. J. Thorn, T. J. Emge, K. Eriks, P. C. Leung, H. H. Wang
Phone: (312)-972-3464
$949,000 02-1

New materials synthesis and characterization focussing on synthetic organic metals, organic superconductors, dielectric materials, and organometallic compounds that behave as model catalysts or catalysts; development of structure-property relationships, and electrical properties measurements, of synthetic metals based on TMTSF (tetramethyltetraselenafulvalene) and BEDT-TTF bis(ethylenedithiotetrathiofulvalene); continuing development of the neutron time-of-flight single-crystal diffractometer (SCD), and the associated U.S. university-industrial users group, at the Intense Pulsed Neutron Source; diffuse scattering and crystal structure studies at the SCD as a function of temperature (10-300 K); development of a facility for single crystal X-ray studies centered around a low temperature (10 K) X-ray instrument for electron density and structural studies.

049. INTENSE PULSED NEUTRON SOURCE PROGRAM (see also page D-7)

G. H. Lander, B. S. Brown, J. M. Carpenter, C. W. Potts,
A. W. Schulke, T. G. Worlton, R. K. Crawford, F. J. Rotella,
M. H. Mueller, C. K. Loong
Phone: (312)-972-5518
$4,900,000 02-1

The IPNS Program has the goal of providing an intermediate-flux pulsed spallation neutron source for condensed matter research with neutron scattering and irradiation techniques. The IPNS facility is equipped with 7 instruments which are regularly scheduled for users and 3 beam tubes which are assigned to special experiments. Routine operation started in November 1981. The facility is run as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 110 experiments, many involving participants in collaborative research from Universities and industry were performed in the period October 1981-October 1983 and another 60 will be scheduled for the next 6 months. Industrial Research on a proprietary basis, which allows the company to retain full patent rights, has been initiated with a number of companies (Schlumberger-Doll, Amoco, Exxon) and is encouraged. Relevant Argonne research programs appear under the neutron activities of the Materials Science and Technology Division of Argonne National Laboratory.

ARGONNE NATIONAL LABORATORY (continued)

050. SUPERCONDUCTIVITY AND MAGNETISM

B. D. Dunlap, G. W. Crabtree, K. E. Gray, D. G. Hinks,
H. A. Kierstead, T. I. Morrison, G. K. Shenoy, K. Aoki,
A. J. Fedro, W. P. Joss, S. K. Malik, B. D. Terris, A. M. Umarji
Phone: (312)-972-5538

$1,391,000 02-2

Experimental and theoretical investigations of the magnetic and superconducting properties of materials; studies of ternary compounds including Chevrel phase and rare-earth rhodium boride materials; electronic and transport studies of organic superconductors; studies of the electronic properties of mixed valence and narrow-band materials containing rare-earth and actinide elements; soft X-ray synchrotron beam-line development; experimental techniques include the de Haas-van Alphen effect, Mossbauer spectroscopy, transport and magnetic measurements, electron tunneling, EELS, NMR, EXAFS and XANES, heat capacity, materials preparation, and characterization.

051. MATERIALS PREPARATION AND CHARACTERIZATION AND FAST ION TRANSPORT IN SOLIDS

S. Susman, T. O. Brun, K. Kuriyama
Phone: (312)-972-5470

$464,000 02-2

Preparation of metal, insulator and semiconductor single crystals with documented physical and chemical properties; solidification of vitreous systems with characterized and reproducible compositions and thermal histories; investigations of mechanisms involved in purification, crystal growth, phase transformations and solidification; materials of current interest include semiconducting chalcogenide glasses, Zintl-phase compounds, complex aluminosilcates and cyanides; basic studies conducted in the microscopics of charge and mass transport in solid electrode and electrolyte materials utilizing X-ray diffraction, nuclear magnetic resonance, ionic conductivity, EXAFS, and optical spectroscopy; fast ion transport examined in mixed electronic and ionic conductors and in fast-ion glasses; these include Li-Al alloys, NASIGLAS, and both crystalline and vitreous eucryptites.

ARGONNE NATIONAL LABORATORY (continued)

052. ELECTRONIC STRUCTURE AND BONDING

D. J. Lam, A. T. Aldred, A. J. Arko, S.-K. Chan, G. S. Knapp,
M. V. Nevitt, B. W. Veal
Phone: (312)-972-4966
$1,500,000 02-2

Experimental and theoretical studies of electronic structure and its relationship to physical and chemical properties and bonding in solids; X-ray photoemission (XPS) and X-ray absorption (XANES and EXAFS) spectroscopic studies of structural and electronic properties of actinide oxides in silicate glasses; crystal chemistry and structural phase transformation studies of complex metal oxides using X-ray diffraction and electron microscopy; XPS and XANES studies of structural and electronic properties of ABO_4 compounds; thermal and lattice properties study of ABO_4 compounds using heat capacity, EXAFS, Raman scattering and ultrasonic measurements; theoretical studies of photoelectron spectra and bonding of ABO_4 and AB_2O_4 compounds; development of molecular cluster code to calculate total energy of embedded oxide clusters; formulation of the theory of EXAFS and XANES for heavy elements; angle resolved photoemission spectroscopy and de Haas-van Alphen studies of the electronic band structure of actinide intermetallic compounds; magnetization and photoemission spectroscopy (UPS and XPS) studies of actinide intermetallic compounds to determine the electronic configuration and stability of 5f electron states.

053. LAYERED AND THIN FILM MATERIALS

I. K. Schuller, S. D. Bader, M. B. Brodsky, M. Grimsditch,
C. S. L. Chun, L. Sill, G. W. Zajac
Phone: (312)-972-5469
$946,000 02-2

Research on the growth and physical properties obtained by thin film techniques--epitaxial films and sandwiches, metallic and insulating superlattices, amorphous metals, and superconductors; preparation techniques include molecular beam epitaxy, evaporation and sputter deposition; materials characterization methods include: X-ray and neutron scattering, low and high energy electron diffraction, and electron microscopy for structural studies; low temperature transport, superconductivity and magnetism; electronic structure studies via AES, UPS, XPS in conjunction with theoretical band structures; elastic, magnetic and vibrational properties using Brillouin and Raman scattering; theory of interface and growth phenomena.

ARGONNE NATIONAL LABORATORY (continued)

054. CONDENSED MATTER THEORY

D. Y. Smith, L. Guttman, R. Kalia, D. Koelling, A. Rahman,
P. Vashishta, K. Lee, M. Norman, M. Schneider
Phone: (312)-972-5481
$902,000 02-3

Condensed matter theory focusing on statistical physics, electronic structure, and the defect solid state. Current areas of study include: molecular-dynamics modeling of structural phase transitions, melting and nucleation, and fast ion transport in solids; electronic structure calculations of organic superconductors and narrow-band materials, including actinides and mixed-valence systems; many-body effects, especially Green's function Monte Carlo simulation of multi-exciton complexes and the electron-hole liquid; optical and X-ray properties of materials; the electronic structure of defects in insulators and electron solvation in molten salts; calculations of the spatial and electronic structure of amorphous semiconductors and covalent glasses.

055. ULTRA-HIGH FIELD SUPERCONDUCTORS

K. E. Gray, R. T. Kampwirth, D. W. Capone II
Phone: (312)-972-5521
$85,000 02-5

Development of magnetron sputtered films of superconducting materials such as NbN for use in magnets operating in the 15-24 Tesla range; effort includes effect of preparation conditions and substrate type on superconducting properties such as critical current density and upper critical field; radiation and strain tolerance will be measured; material characterization by X-ray, EELS, RBS, and TEM; technique development for fabrication of continuous tapes and/or wires of stabilized NbN suitable for winding ultra-high field superconducting magnets.

056. GEOPHYSICAL PROSPECTING WITH SQUIDS

R. T. Kampwirth
Phone: (312)-972-5521
$100,000 02-5

Development of portable instrumentation system for data acquisition and analysis of extremely weak magnetic and electric fields using Superconducting QUantum Interference Devices (SQUIDs) and telluric electrodes for signal detection; both magnetotelluric and controlled source signal sources; applications include nonintrusive lithosphere mapping, and search for subsurface hydrocarbon and mineral deposits; especially useful in regions of high sound velocity (e.g., basaltic overflows) where no seismic sections are obtainable; instrumentation system being prepared for transfer to an institution doing geophysics research.

ARGONNE NATIONAL LABORATORY (continued)

057. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

M. Blander, R. Blomquist, L. A. Curtiss, H. E. Flotow,
V. A. Maroni, P. A. G. O'Hare, M.-L. Saboungi
Phone: (312)-972-4548
$810,000 03-2

Experimental and theoretical studies of thermodynamic and structural properties of ordered solutions, amorphous (metastable) materials, strategic minerals, and chemical species that have significance for elevated-temperature corrosion processes; thermodynamic measurements (e.g., emf), structural (e.g., neutron diffraction) and theoretical (e.g., molecular dynamics) studies of solution behavior of ordered and associated liquids (e.g., chloroaluminates, ionic alloys, silicates); thermodynamic calculations based on statistical mechanics of complex metallurgical media as well as corrosion processes; electronic absorption spectroscopy, X-ray diffraction, proton activation, and cyclic voltammetry are used to explore the dissolution of metals contained in domestic minerals and in industrial/energy by-products; thermochemical measurements of enthalpies of formation, standard entropies, and Gibbs energies of formation of strategically important minerals, fiber optic materials, and fast ion conducting glasses; drop calorimetric and vapor pressure measurements on systems exhibiting metal-to-nonmetal transitions.

058. INTERFACIAL MATERIALS CHEMISTRY

V. A. Maroni, M. Blander, L. A. Curtiss, B. D. Holt, S. A. Johnson,
R. Kumar
Phone: (312)-972-3513
$1,017,000 03-2

Experimental and theoretical investigations of interfacial processes that are important to corrosion science, catalysis, and atmospheric chemistry; studies of surface and near-surface gas/particle and gas/substrate interactions using attenuated total internal reflection (ATR) Fourier transform infrared spectroscopy; ATR and Auger/ESCA studies of bonding of absorbed species in the cavities of shape selective catalysts; Ab-initio quantum mechanical and classical statistical mechanical calculations of structure, bonding, and reaction energies with emphasis on surface absorbed species and atomic clusters; investigations of the mechanism of conversion of SO_2 to sulfates in the atmosphere using oxygen isotopic techniques and high-resolution tunable diode laser infrared spectroscopy.

ARGONNE NATIONAL LABORATORY (continued)

059. AQUEOUS CORROSION

V. A. Maroni, D. M. Gruen, C. A. Melendres, Z. Nagy, M. Pellin,
R. M. Yonco
Phone: (312)-972-3513

$150,000 03-2

Fundamental aspects of aqueous corrosion with emphasis on mechanisms responsible for stress corrosion cracking (SCC) of iron and iron-based alloys at high temperatures and pressures (300°C, 100 atm); application of in-situ surface-sensitive spectroscopic techniques (laser Raman, Raman gain, second harmonic generation, surface extended X-ray absorption fine structure, and Auger/ESCA) in combination with transient electrochemical methods to unravel the details connecting surface adsorption/reaction initiation and grain boundary effects involved in SCC; supporting theoretical studies using (1) molecular dynamics methods to study interactions at the water-metal interface on the molecular level and (2) porous electrode theory to obtain a macroscopic description of the influence of water chemistry on the corrosion behavior of iron-based alloys.

060. PARTICLE-SURFACE INTERACTION CHEMISTRY AND CATALYSIS

D. M. Gruen, B. M. Abraham, W. F. Calaway, L. E. Iton,
A. R. Krauss, G. J. Lamich, C. A. Melendres, M. H. Mendelsohn,
M. J. Pellin, C. E. Young
Phone: (312)-972-3513

$1,022,000 03-3

Surface analysis by resonance ionization of sputtered atoms (SARISA) using pico-coulomb ion fluences combined with direct detection techniques; adsorbate structures, velocity and excited state distributions of sputtered species; mechanism of radiation-enhanced surface segregation in dilute alloy systems; synthesis of new shape-selective, catalysts incorporating small metal clusters; characterization and evaluation of catalysts using NMR, EPR, PAS, DTA, and Berty reactor techniques; electronic structure of matrix-isolated ligand-free transition metal clusters by laser fluorescence spectroscopy; electrocatalysis of O_2 reduction on metal-porphyrin and phthalocy-anine-coated electrode surfaces; dependence on pH of the viscosity and of the instantaneous and static shear moduli of biological surfactant monolayers.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Metallurgy and Materials Science Division - 01 -

A. N. Goland - Phone (FTS) 666-3819 or 516-282-3819
M. Suenaga - Phone (FTS) 666-3518 or 516-282-3518

070. BASIC PROPERTIES OF AMORPHOUS SEMICONDUCTING MATERIALS

P. E. Vanier, R. R. Corderman, F. J. Kampas
Phone: (FTS) 666-3535 or (516)-282-3535
$290,000 01-1

Investigations of the growth, structure, and properties of plasma-deposited thin-film amorphous semiconductors. Studies by optical and mass spectroscopy of processes in the plasma and their relation to film growth and defect formation. Studies of film structure and morphology by electron and optical microscopy, positron annihilation, and EXAFS. Studies of chemical bonding by infrared absorption and electron spin resonance. Measurement of photoelectronic properties and their correlation with structural and bonding characteristics.

071. MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS

H. S. Isaacs, K. Sieradzki, R. C. Newman, N. Bandyopadhyay
Phone: (FTS) 666-4516 or (516)-282-4516
$400,000 01-2

✓ Experimental studies of brittle fracture of ductile metals and alloys during stress-corrosion cracking; role of thin surface films, correlation of acoustic and electrochemical noise during cracking with crack arrest marks, intergranular stress-corrosion cracking of Fe-P alloys. Molecular dynamic and analytic modeling of environmentally induced fracture processes. Modeling and experimental studies of initiation of localized corrosion and electrical and structural properties of passive oxide layers; measurement of the electrochemistry within localized sites using a scanning vibrating probe to determine current distributions.

072. SUPERCONDUCTING MATERIALS

D. O. Welch, M. Suenaga, J. Tafto, N. Higuchi
Phone: (FTS) 666-3517 or (516)-282-3517
$420,000 01-3

Fundamental properties of high critical temperature and critical field superconductors; effects of strain, disorder, and lattice defects on superconducting properties; theoretical models of interatomic forces, lattice defects, and diffusion kinetics in A15 compounds; annealing and layer growth kinetics in A15 compounds; studies by electron microscopy of lattice defects in superconducting compounds; flux pinning; properties of composite superconductors; new methods of fabricating superconducting materials.

BROOKHAVEN NATIONAL LABORATORY (continued)

073. PHYSICAL PROPERTIES OF METAL-INTERSTITIAL SYSTEMS

M. S. Pick (on leave), T. H. Metzger, S. M. Heald, D. O. Welch
Phone: (FTS) 666-3517 or (516)-282-3517
$500,000 01-3

Studies of physical and metallurgical factors which influence the behavior of interstitial solutes in metals and alloys; studies of the role of microstructure, lattice defects, alloying effects, and surface properties on the thermodynamics, kinetics, and mechanisms of hydrogen uptake and release in transition metals, solid solutions, and intermetallic compounds; effect of dissolved hydrogen upon fracture strength; structural and microstructural studies of metal-interstitial systems using optical, neutron, and X-ray diffraction, EXAFS, electron microscopic, nuclear depth profiling, and surface sensitive techniques; statistical mechanics of metal-interstitial systems.

074. ELECTROCHEMICAL PROPERTIES OF INTERFACES

W. E. O'Grady
Phone: (FTS) 666-2829 or (516)-282-2829
$50,000 01-3

Studies of the role played by the structure, chemical composition, and oxidation states of the surface in electrode reactions using electrochemical techniques combined with low energy electron diffraction, Auger electron spectroscopy, X-ray photoelectron spectroscopy, and EXAFS.

075. PROPERTIES OF DEFECTS IN MATERIALS

C. L. Snead Jr.
Phone: (FTS) 666-3502 or (516)-282-3502
$300,000 01-4

Effects of different types of irradiation on critical properties of type-II superconductors; electron, reactor neutron, 14-MeV neutron, 17-MeV, 800-MeV and 30 GeV proton irradiations; Nb-Ti, and A15 superconductors; defect and microstructure changes in irradiated materials; application of positron annihilation to defect studies; irradiation-induced defects and gases in metals. Mechanical properties of various materials using internal friction and dynamical Young's modulus techniques; study of hydrogen in metals and martensitic transformations.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

Department of Chemistry - 02 -

A. P. Wolf: (FTS) 666-4397 or 516-282-4397

076. NEUTRON SCATTERING

L. M. Corliss, J. M. Hastings, R. Thomas
Phone: (FTS)-666-4376 or (516)-282-4376
$420,000 02-1

Neutron scattering studies of the statistical mechanics of phase transitions, the dynamical properties configurations of magnetic materials, and also crystal structures where relevant. The measurement of the spatial distribution of magnetization and the behavior of spontaneous fluctuations, both of which are essential to understanding magnetic phase diagrams and associated first- and second-order transitions. Because of the universal nature of critical phenomena, information gained from magnetic systems benefit studies of other systems exhibiting second-order phase transformations, such as simple and multicomponent liquids, alloy systems, and superfluids.

Department of Physics - 02 -

V. J. Emery: (FTS) 666-3765 or 516-282-3765

077. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

S. M. Shapiro, J. D. Axe, D. P. Belanger, P. Böni, J. P. Wicksted, H. Yoshizawa
Phone: (FTS) 666-3822 or (516)-282-3822
$1,145,000 02-1

Neutron scattering studies of the structure and dynamics of phase transitions. Random magnetic systems, magnetic superconductors, low dimensional charge density waves, incommensurate systems and soft modes in solids.

078. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES

G. Shirane, B. H. Grier, C. F. Majkrzak, L. Passell, S. K. Satija, O. Steinsvoll, J. P. Wicksted, Y. J. Uemura
Phone: (FTS) 666-3732 or (516)-282-3732
$1,490,000 02-1

Neutron scattering studies of low-lying excitations in solids and overlayer films, electron-phonon interactions in metals and lattice dynamics of metal hydride systems. Development of efficient neutron polarizer and new devices for beam modulation.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

079. X-RAY SCATTERING RESEARCH

D. E. Moncton, K. D'Amico, B. C. Frazer (on leave), L. D. Gibbs,
H. Moudden
Phone: (FTS)-666-2741 or (516)-282-2741
$900,000 02-2

Structural and dynamic properties of condensed matter systems, studied by x-ray and neutron scattering; phase transition and new states of matter particularly in two-dimensional (2D) systems: 2D melting, commensurate-incommensurate transitions; reconstruction, and molecular orientational transitions. Extension to single crystal surfaces under ultra high vacuum conditions is in progress; studies of the possibilities for magnetic x-ray scattering study of the structure of atomic microclusters produced in nozzle beams; research and development studies of synchrotron instrumentation for NSLS experiments.

080. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

K. G. Lynn, D. Chen (CCNY), D. Fischer (SUNY-Stony Brook),
W. Frieze, D. Gidley (Bell Labs), C. Lewis (DAS), B. Nielsen,
L. Roelling (CCNY), C. L. Snead Jr. (DAS), M. Weber (CCNY)
Phone: (FTS) 666-3710 or (516)-282-3710
$955,000 02-2

Investigations of perfect and imperfect solids and their surfaces by newly developed experimental methods; use of both magnetically and electrostatically focussed variable energy positron beams coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron Diffraction, Photoemission, Thermal Desorption Spectroscopy); high resolution positron energy loss measurements of adsorbed molecules on metal surfaces, surface state lifetimes, positron diffusion lengths, positron work functions, positronium formation with measurement of its emitted energy distribution, metal-metal and metal-insulator interface and ion implanted and laser annealed semiconductors; use of recently developed SR channel at AGS.

081. ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION

D. E. Cox, K. G. Lynn, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516)-282-3818/3870
$460,000 02-2

Preparation and characterization of inorganic materials by high temperature, sputtering and solution techniques, crystal orientation; development and application of profile methods for structural analysis of neutron and x-ray powder diffraction data; application of synchrotron radiation to high resolution powder diffractometry.

BROOKHAVEN NATIONAL LABORATORY (continued)

082. THEORETICAL RESEARCH

P. Bak, S. Coppersmith, J. Davenport, G. J. Dienes, V. J. Emery,
Y. Shapir, R. M. Sternheimer, G. Vineyard, R. E. Watson, M. Weinert
Phone: (FTS) 666-3798 or (516)-282-3798
$660,000 02-3

Phase transitions, critical and cooperative phenomena in magnetic systems, organic metals and incommensurate structures; properties of one- and two-dimensional materials by analytic and numerical methods; nonlinear systems; metal surfaces and adsorbed films; electronic structure of metals and alloys; x-ray and neutron scattering; properties of disordered materials and crystal defect physics; high pressure, high temperature properties of solids.

083. SURFACE PHYSICS RESEARCH

M. Strongin, S. Hulbert, P. D. Johnson, V. J. Murgai, S. Raeen,
D. Wesner
Phone: (FTS) 666-3763 or (516)-282-3763
$850,000 02-5

Synchrotron Radiation as a technique to study the geometrical and electronic properties of surfaces and interfaces. Special emphasis has also been given to the development of new spectroscopies such as inverse photoemission and the construction of an undulator beam line at NSLS to enable experiments on spin polarized photoemission. Support has also been given to the development of low-temperature techniques which can be used at NSLS. The problems presently being studied include: a) electronic properties of overlayers and clean metal surfaces, and hydrogen on metal surfaces. Besides valence band photoemission, inverse photoemission and core level spectroscopy are used as tools in this area; b) organic molecules on surfaces and properties of organic solids; c) surface metallurgy and surface compounds; d) cooperative effects and phase transitions in adsorbate layers on metal surfaces. In particular, studies of phase transitions of Xe layers on metal surfaces: e) properties of ion implanted surfaces; f) studies of metal clusters in rare gases and in organic solids; g) studies of oxidation and other chemical reactions at low temperatures.

BROOKHAVEN NATIONAL LABORATORY (continued)

High Flux Beam Reactor - 02 -

G. C. Kinne - Phone (FTS) 666-4061 or 516-282-4061
D. C. Rorer - Phone (FTS) 666-4056 or 516-282-4056

084. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS

G. C. Kinne, D. C. Rorer, M. H. Brooks, R. C. Karol, D. G. Pitcher, O. Jacobi, S. Protter, L. Junker, P. Tichler, J. Detweiler, W. Brynda
Phone: (FTS) 666-4061 or (516)-282-4061
$6,900,000 02-1

Operation of the High Flux Beam Reactor, including routine operation and maintenance of the reactor, procurement of the fuel, training of operators, operation and maintenance of a liquid hydrogen moderated cold neutron source, and irradiation of samples for activation analysis, isotope production and radiation damage studies. Technical assistance provided for experimental users, especially with regard to radiation shielding and safety review of proposed experiments. Additionally, planning and engineering assistance provided for projects for upgrading the reactor.

National Synchrotron Light Source - 02 -

M. Blume: (FTS) 666-3735 or (516)-282-3735

085. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT (see also page D-1)

M. Blume, M. Barton, K. Batchelor, R. Blumberg, J. Galayda,
J. Godel, J. Hastings, H. Hsieh, R. Klaffky, S. Krinsky, A. Luccio,
C. Pellegrini, W. Thomlinson, A. van Steenbergen, G. Williams
Phone: (FTS) 666-3735 or (516)-282-3735
$7,300,000 02-2

Support of operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers operation and maintenance of the two NSLS electron storage rings and the associated injector combination of linear accelerator-booster synchrotron; operation and maintenance of the photon beam lines of the vacuum ultraviolet (VUV) and X-ray storage rings; and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon lines of the facility by means of new developments in high resolution photon optics, state-of-the-art monochromators, X-ray mirror systems, detectors and other necesary instrumentation. The NSLS storage rings will provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources.
This facility is the first in this country to be designed expressly for use of synchrotron radiation. An extensive research and development program is necessary in order to optimize performance characteristics and also to develop new beam line instrumentation which will permit users to take full advantage of the unique research capabilities offered by this facility. This research and development effort also supports the construction of the beam lines and devices funded under the Phase II construction project.

LABORATORIES

IDAHO NATIONAL ENGINEERING LABORATORY
550 2nd Street
Idaho Falls, Idaho 84301

Materials Science Division - 01 -

D. D. Keiser - Phone (FTS) 583-1770 or (208) 526-1770

100. MATERIALS SCIENCE WELDING RESEARCH

J. F. Key, H. B. Smartt, M. E. McIlwain, G. R. Smolik
Phone: (FTS) 583-8332 or (208)-526-8332
$550,000 01-5

Establishment of quantitative relationships between materials and processes used to weld them. Emphasis on predicting structure and properties of a weldment from process parameters and materials chemistry. Heat source/molten pool interaction investigations utilizing high-speed cinematography, emission spectroscopy, laser-induced fluorescence spectroscopy, holographic interferometry, infrared thermography, and finite element (and difference) computer modeling. Solidification and microstructure/properties correlations utilizing infrared thermography, high-speed x-radiography, optical and electron microscopy, calorimetry, and computer modeling. Technology transfer through American Welding Technology Applications Center.

LABORATORIES

ILLINOIS, UNIVERSITY OF
at Urbana-Champaign
Urbana, Illinois 61801

Materials Research Laboratory
C. P. Flynn - Phone: (217) 333-1370

105. EFFECT OF FLUID FLOW ON LOCALIZED CORROSION

R. C. Alkire
Phone: (217)-333-0063
$70,000 01-1

Corrosion of passivating systems. Mechanisms of corrosion pit formation. Transport, kinetics and convective diffusion at localized corrosion sites. Erosion, cavitation, pitting, repassivation, and transient metal salt films. Corrosion inhibition.

106. CENTER FOR MICROANALYSIS OF MATERIALS (see also page D-19)

J. A. Eades, C. Loxton, J. Woodhouse
Phone: (217)-333-8396, (217)-333-0386, or (217)-333-3888
$240,000 01-1

Chemical, physical and structural characterization of materials. Surface and bulk microanalysis. Electron microscopy, X-ray diffraction, Auger spectroscopy, SIMS and other techniques. Collaborative research programs.

107. RAPID SOLIDIFICATION PROCESSING

H. L. Fraser
Phone: (217)-333-1975
$165,000 01-1

Development of rapid solidification processing of alloys with powder preparation by laser, spin and centrifugal atomization and subsequent consolidation by dynamic compaction technqiues. Characterization of microstructure and measurement of properties developed by heat treatments. Understanding structure-property relationships, mechanisms of metastable phase formation and transformations.

108. SEMICONDUCTOR CRYSTAL GROWTH BY ION BEAM SPUTTERING

J. E. Greene
Phone: (217)-333-0747
$150,000 01-1

Mechanisms and kinetics of crystal growth. Metastable single crystal alloys for solar and optical applications. Ion beam sputtering, molecular beam epitaxy, laser heating and low energy ion bombardment methods applied to III-V based compounds and III-IV-V_2 chalcopyrite systems.

ILLINOIS, UNIVERSITY OF (continued)

109. GRAIN GROWTH IN ALUMINA

D. S. Phillips
Phone: (217)-333-6440
$70,000 01-1

Characterization of grain boundaries in solid-state and liquid-phase sintered aluminas by transmission electron and analytical electron microscopy. Correlation of boundary mobilities with microstructures.

110. PROCESSING AND CHARACTERIZATION OF NOVEL AMORPHOUS MATERIALS AND SURFACES

J. M. Rigsbee
Phone: (217)-333-6584
$55,000 01-1

Laser processing to modify structure, composition and physical properties of metallic and ceramic surfaces. Erosion and abrasion resistant surfaces. Physical vapor deposition studies of metastable $Cu_xCr_{(1-x)}$ alloys.

111. MICROCHEMISTRY OF SOLIDS

C. A. Wert
Phone: (217)-333-1440
$65,000 01-1

Development of microanalytic methods for sulfur in coal. Studies of changes in pyrite, pyrrhotite and organic sulfur content during coal treatment and conversion.

112. PROCESSING AND MICROSTRUCTURE OF COMPLEX CERAMIC SYSTEMS

A. Zangvil
Phone: (217)-333-6829
$85,000 01-1

Microstructure and microchemistry of SiC-AlN, SiC-BeO, SiC-BN and SiC. Effect of processing variables and additives on the structure and microchemistry of ceramic systems. Hydrogen effects in SiC. Role of chemistry in the formation of polytypes.

113. HYDROGEN BEHAVIOR IN BCC METALS

H. K. Birnbaum
Phone: (217)-333-1901
$130,000 01-2

Mobility of hydrogen and deuterium in b.c.c. metals such as niobium. Gorsky Effect, stress induced reorientation, piezoresistance, acoustic techniques used to study low temperature mobility and interaction of hydrogen with trapping sites. Behavior of hydrogen at surfaces and transfer of hydrogen across surfaces. Phase transitions in the high concentration metal-hydrogen alloys studied with X-rays, neutrons, and acoustic techniques.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

114. MICROMECHANICS AND MICROMECHANISMS OF FRACTURE

H. K. Birnbaum, C. J. Altstetter, F. A. Leckie, R. M. McMeeking,
D. Socie, J. F. Stubbins
Phone: (217)-333-1901

$270,000 01-2

Fracture mechanics and microstructural studies of the fundamental mechanisms of fracture are applied to metals and ceramics. Environmental effects on the fracture of alloys of Fe, Ni, Al, Ti, Al_2O_3-ZrO_2, MgO using HVEM. Role of phase transitions in fracture of hydride forming systems and stainless steels. Effects of environment on dislocation behavior and plasticity related fracture. High temperature corrosion and scaling. Fatigue and fracture under multiaxial loading and the role of microstructural changes. Development of damage and failure criteria for systems undergoing phase transitions and enhanced plasticity.

115. COUNCIL ON MATERIALS SCIENCE

D. Lazarus
Phone: (217)-333-0492

$75,000 01-2

Study and analysis of current and proposed basic research programs on materials and assessment of their relevance to problems of energy utilization. Consideration of national facilities needs. Convening of panel studies on selected topics.

116. STRUCTURE, CRACKING AND CHEMISTRY OF CERAMIC GRAIN BOUNDARIES AND PHASE BOUNDARIES

S. D. Brown, A. Zangvil
Phone: (217)-333-4766 or (217)-333-6829

$65,000 01-2

Effects of impurities on structure and chemistry of regions contiguous to grain boundaries in SiC and Si_3N_4. Delayed failure, fracture toughness, creep and corrosion. Emphasis on effects of partial pressures of hydrogen on strength properties. Structure of AlN-SiC solid solutions.

117. PHYSICAL PROPERTIES OF CERAMIC MATERIALS

W. S. Williams
Phone: (217)-333-3524

$100,000 01-2

Deformation characteristics of diborides and non-stoichiometric monocarbides of IVb and Vb transition metals at extremely high temperatures. Dislocation properties, second phase precipitates, and their role in diffusion limited flow stress. Microchemical analysis of precipitates, grain boundaries and stacking faults by EELS.

ILLINOIS, UNIVERSITY OF (continued)

118. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE AND BOROSILICATE GLASSES

H. Chen
Phone: (217)-333-7636
$80,000 01-3

Investigation of devitrification kinetics and associated microstructural and compositional changes in silicate and borosilicate based glasses containing metal oxides using EXAFS, small and wide angle x-ray scattering and SEM methods. Mechanisms of metal-silicide thin film formation. Kinetics of layer growth.

119. DIELECTRIC SOLIDS

D. A. Payne
Phone: (217)-333-2937
$120,000 01-3

Synthesis, powder preparation, crystal growth, forming methods, materials characterization and property measurements on electrical and structural ceramics. Sol-gel processing of thermal barriers and mechanical coatings. Chemical, electrical and mechanical boundary conditions in polarizable deformable solids, twin and domain structures, ferroelasticity and crack propagation. Amorphous ferroelectrics.

120. MICROSTRUCTURE AND CRYSTALLIZATION IN NOVEL GLASSY SYSTEMS

S. H. Risbud
Phone: (217)-333-2885
$90,000 01-3

Glass synthesis and phase transformations in quasi-binary II-IV-V2 semiconducting glasses. Electrical, optical and thermomechanical properties of these glasses. Melting, solidification, and glass formation in quasi-binary systems of the Cd-Zn-Ge-As system. Location of N in crystallized glasses. Formation of glass-ceramic composites.

121. MICROWAVE STUDIES OF TUNNELING STATES IN DISORDERED MATERIALS

H. J. Stapleton
Phone: (217)-333-0073
$100,000 01-3

Effects of tunneling states and disorder in amorphous semiconductors, fast ionic conductors, glasses, and crystals using electron spin relaxation, electron spin resonance, electron-nuclear double resonance, and microwave susceptibility in the 0.25-25 K temperature range.

ILLINOIS, UNIVERSITY OF (continued)

122. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS

A. C. Anderson
Phone: (217)-333-2866
$120,000 02-2

Experimental studies of glassy metals, of fast ion conductors, of polymers, composites and ceramics, and of irradiated or deformed ionic and other crystals; influence of defects and disorder on macroscopic properties including specific heat, magnetic susceptibility, thermal and electrical transport, thermal expansion, and ultrasonic and dielectric dispersion at 0.02-200K.

123. PHOTOEMISSION STUDIES OF THE ELECTRONIC STRUCTURE OF SURFACES AND INTERFACES

T.-C. Chiang
Phone: (217)-333-2593
$150,000 02-2

Synchrotron radiation photoemission studies of electronic structure of semiconductor surfaces and interfaces prepared in-situ by molecular beam epitaxy; adsorption kinetics and catalysis on surfaces; properties of alloy surfaces.

124. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION

J. D. Dow
Phone: (217)-333-2981
$40,000 02-2

Theory of synchrotron radiation spectra of deep cores in metals and semiconductors. Theory of semiconductor surface states. Theory of surface reconstruction geometries of semiconductors. Theory of disordered systems and alloys.

125. THE USE OF VERY HIGH PRESSURE TO INVESTIGATE THE ELECTRONIC STRUCTURE OF MATTER

H. G. Drickamer
Phone: (217)-333-0025
$170,000 02-2

Studies of the pressure tuning of electronic energy levels with emphasis on optical absorption measurements including absorption edges, metal cluster compounds and charge transfer phenomena, as well as semiconductor-metal interfaces.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

126. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS

L. R. Faulkner
Phone: (217)-333-8306
$10,000 02-2

Exciton propagation from absorbing chromophores in polymer films to trapping sites on film surfaces at monolayer coverage. Controlled molecular assemblies of three dimensional reaction systems.

127. HIGH-FIELD SUPERCONDUCTORS

D. M. Ginsberg
Phone: (217)-333-4356
$70,000 02-2

Investigation of high-field superconductors by preparation and detailed characterization of samples and by measurements of critical magnetic field, specific heat, Raman effect, magnetic susceptibility, neutron diffraction, and transport properties.

128. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER

A. V. Granato
Phone: (217)-333-2639
$150,000 02-2

Investigation by ultrasonic methods of impurity - self interstitial interactions in electron irradiated metals and semiconductors, and of hydrogen in bcc metals.

129. DEFECT AND ELECTRONIC PROPERTIES OF SOLIDS

D. Lazarus
Phone: (217)-333-0492
$25,000 02-2

Atomic mobility and electrical conduction in solid electrolytes and metallic glasses, studied as a function of temperature and pressure. Mainly concerned with elucidating atomistic defect formation and jump processes.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

130. PROPERTIES OF CRYSTALLINE CONDENSED GASES

R. O. Simmons, V. R. Pandharipande
Phone: (217)-333-3760 or (217)-333-8079
$190,000 02-2

Measurement and theory of momentum density in bcc, hcp, and liquid helium; pulsed neutron scattering; phase transitions and structure determination in solid hydrogen by neutron diffraction; isotopic phase separation in solid helium; thermal and isotopic defects in helium crystals; quantum effects in diffusion.

131. NUCLEAR MAGNETIC RESONANCE IN SOLIDS

C. P. Slichter
Phone: (217)-333-3834
$170,000 02-2

Investigations of layered materials and one dimensional conductors with charge density waves, of platinum-alumina reforming hydrocarbon catalysts, and of spin glasses using nuclear magnetic resonance methods.

132. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS

H. Zabel
Phone: (217)-333-2514
$150,000 02-2

X-ray and neutron scattering investigations of structural, thermal and vibrational properties of alkali metal graphite-intercalation compounds; staging, dislocations, point defects, phonon dispersion, order-disorder transformations, and diffusion. Microstructural properties of metal and semiconductor MBE grown superlattices.

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Materials and Molecular Research Division

A. W. Searcy - Phone: (415) 486-6062 or FTS: 451-6062

140. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES

R. Gronsky
Phone: (FTS) 451-5674 or (415)-486-5674
$170,000 01-1

Transformation interfaces include homophase boundaries, heterophase boundaries and "free" surfaces at which solid state reactions are either initiated or propagated. The atomic configurations of such interfaces and the establishment of the relationship between their structure and relevant interfacial properties. Correlations between the segregation behavior, precipitation behavior and deformation behavior of interfaces and their detailed defect structures. Experiments are chiefly by transmission electron microscopy, including energy dispersive X-ray and electron energy loss spectroscopies; results are correlated with theoretical predictions of interfacial phenomena.

141. DESIGN, MICROSTRUCTURE, AND PROPERTIES OF ALLOYS: INORGANIC MATERIALS

G. Thomas
Phone: (FTS) 451-5656 or (415)-486-5656
$580,000 01-1

A multicomponent, interdisciplinary program in physical metallurgy and ceramics involving fundamental quantitative studies of the structure-property relationships in technologically significant materials involved in energy and conservation. Characterization of both structure and composition at the highest levels of spatial (transmission electron microscopy) and chemical (spectroscopy) resolutions. Specific tasks include: a.) dual phase, ferrite-martensite steels for rod and wire, optimization of microstructure and processing, analytical studies of solute partitioning, fatigue, and wear; b.) martensitic and bainitic steels, fundamental studies of phase transitions, relation to wear; surface treatments (laser technology), grain boundary precipitation, effect of copper; c.) magnetic materials; structure of audio recording tape, piezoelectric materials, rare-earth alloys.

LAWRENCE BERKELEY LABORATORY (continued)

142. SOLID STATE PHASE TRANSFORMATION MECHANISMS

K. H. Westmacott
Phone: (FTS) 451-5663 or (415)-486-5663
$190,000 01-1

Factors that govern phase changes and phase stability in order to facilitate first principle alloy design. Advanced electron optical techniques, especially high voltage and high resolution electron microscopy. The relationship between lattice defects and precipitate phase growth. Crystallographic theory of precipitation with a parallel experimental program.

143. NATIONAL CENTER FOR ELECTRON MICROSCOPY (see also page D-28)

G. Thomas
Phone: (FTS) 451-5656 or (415)-486-5656
R. Gronsky
Phone: (FTS) 451-5674 or (415)-486-5674
K. H. Westmacott
Phone: (FTS) 451-5663 or (415)-486-5663
$1,090,000 01-1

Organization and operation of a national, user-oriented resource for transmissision electron microscopy. Maintenance, development and application of specialized instrumentation including an Atomic Resolution Microscope (ARM) for ultrahigh resolution imaging, a 1.5 MeV High Voltage Electron Microscopy (HVEM) with capabilities for dynamic in-situ observations, analytical electron microscopes for micromechanical analysis and support facilities for specimen preparation, image analysis, image simulation and instrument development.

144. IN-SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY

J. W. Evans
Phone: (415)-642-3807
$105,000 01-1

Kinetics of reactions between gases and solids; the role of microstructure. Relations between the sites for nucleation and growth of second phases and microstructural features such as microcracks, grain boundaries and dislocations. Environmental cell experiments in the high voltage transmission microscope.

LAWRENCE BERKELEY LABORATORY (continued)

145. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS

D. de Fontaine
Phone: (415)-642-8177
$105,000 01-1

Fundamental investigation of ordering and phase separation in certain metallic alloys. Both theoretical and experimental aspects for the three following topics: atomic ordering in systems exhibiting the phenomenon of long-period superstructure formation; the theoretical tool being primarily the newly developed cluster variation method of statistical thermodynamics; the experimental tool being high-resolution electron microscopy. Phase separation in systems exhibiting partitioning of substitutional and interstitial alloying elements, such as alloy steels; the theoretical tool here being multicomponent nucleation theory and the experimental one being transmission electron microscopy with full analytical capabilities. The interaction of magnetic and ionic ordering in AuFe alloys which exhibit the spin glass phenomenon; the theoretical tool is a modification of the cluster variation method, the experimental one that of high-resolution transmission electron microscopy and diffraction.

146. COLLABORATIVE RESEARCH BY TRANSMISSION ELECTRON MICROSCOPY

A. W. Searcy
Phone: (FTS)451-6062 or (415)-486-6062
$50,000 01-1

This program has been established to foster collaborative research between scientists with specialized skills in advanced techniques of transmission electron microscopy and scientists from other disciplines with projects requiring sophisticated microstructural characterization. Under the program, postdoctoral, or more mature visiting electron microscopists spend up to one year at LBL using the unique instrumentation available at the National Center for Electron Microscopy in (NCEM) collaborative programs with Materials and Molecular Research Division Investigators recommended for support by the NCEM Steering Committee.

147. THEORETICAL PROBLEMS IN ALLOY DESIGN

J. William Morris Jr.
Phone: (FTS) 451-6482 or (415)-486-6482; (415)-642-3815
$540,000 01-2

A multifaceted program of metallurgical research on the science of alloy design. Specific research tasks include: (1) theoretical research on phase transformations in solids and on the influence of microstructure on engineering properties; (2) experimental research on fundamental problems in metallurgy, including the control of microstructure through thermomechanical processing, the influence of microstructure on engineering properties, and the development of probative materials testing techniques; (3) the development of new structural alloys for advanced energy systems, a task mainly concerned with the design of improved structural alloys for low-temperature use; (4) welding metallurgy, including the development of appropriate weld filler metals and weld microstructures to maintain toughness in high strength welded alloys; (5) the development of improved superconducting wires for use in high field superconducting magnets.

148. MECHANICAL PROPERTIES OF CERAMICS

A. G. Evans
Phone: (415)-642-7347
$305,000 01-2

The development of predictive capabilities for the high temperature failure of ceramics and for microstructure/defect development during sintering. Elevated temperature failure studies are concerned with the initiation, growth and coalescence of cracks during creep. Experimental measurements are being correlated with theoretical models containing the dominant microstructural variables. Sintering studies are examining the processes that dictate the presence of retained porosity and defects during solid state and liquid phase sintering.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

149. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS

R. O. Ritchie
Phone: (FTS) 451-5798 or (415)-486-5798; (415)-642-0417
$240,000 01-2

A program to examine the respective roles of mechanical, micromonotonic and cyclic growth of flaws in engineering materials. Current emphasis is being devoted: i) to defining the role of environment and microstructure on microscopic crack closure mechanisms and their effect on subsequent near-threshold fatigue growth of long and short cracks in steels below 10^{-5} mm/cycle, for inert, gaseous, aqueous and viscous environments; ii) to the modelling of crack growth toughness. Characterization of macroscopic growth rate behavior and microscopic failure mechanisms using fracture mechanics, microstructural and surface chemistry (e.g., Auger and ESCA) analysis and detailed fractography.

150. INTERFACES AND CERAMIC MICROSTRUCTURES

J. A. Pask
Phone: (415)-642-3821
$10,000 01-3

Kinetics and mechanisms of solid-state reactions, nucleation and growth phenomena, and distribution of phases in multiphase ceramic systems whose principal phase constituents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with a liquid phase. Mechanisms of corrosion of ceramic materials. Thermodynamics and kinetics of electrochemical reactions at glass-metal interfaces.

151. HIGH-TEMPERATURE REACTIONS

A. W. Searcy
Phone: (FTS) 451-6062 or (415)-486-6062
$295,000 01-3

Emphasis on endothermic decomposition reactions. A general theoretical analysis of decomposition reaction kinetics; a systematic investigation of the separate influences of temperature, product gas pressure, thermal energy balance, particle size, sample size, and catalysts on decomposition rates and on the structure and properties of solid-reaction products; TEM studies of prototype decomposition reactions. Vapor transport through porous solids to obtain quantitative data on high-temperature surface diffusion; theoretical and experimental studies of surface thermodynamics, chemisorption and surface-transport processes.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

152. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS

J. Washburn
Phone: (FTS) 451-6254 or (415)-486-6254
$330,000 01-3

A research program is to advance the understanding of structural defects including the structure of interfaces in semiconductor materials. Particular emphasis on interfaces and defects that are formed during processing steps used for state-of-the-art, solid-state-device manufacture such as ion implantation, oxidation, and contact formation. Studies of the crystalline-to-amorphous transformation during ion damage in silicon and gallium arsenide; an investigation of the detailed mechanisms of crystal growth into amorphous zones; and a study of the growth of Cu_2S layers on the surface of CdS. High-resolution lattice-imaging electron microscopy combined with computer simulation of the images to reveal and interpret fine-scale defects and interface structures, in conjunction with complementary observations such as Rutherford backscattering measurements, secondary ion mass spectroscopy, and electrical or optical measurements.

153. CHEMICAL PROPERTIES AND PROCESSING OF REFRACTORY CERAMICS

L. C. De Jonghe
Phone: (FTS) 451-6138 or (415)-486-6138
$250,000 01-3

Studies of the reactions at ceramic/metal interfaces and their effect on the physical properties of such interfaces. Two different reaction types are considered: Gaseous reduction of transition metal oxides; and subscale oxidation of Ni/ZrO_2 interfaces. Thermogravimetrical analysis, and electron microscope methods to characterize the reaction mechanisms. Acoustic emission detection during thermal cycling to assess the integrity of the metal/ceramic joint. Reactions in the solid state during densification in the $CaO-Al_2O_3$ system.

154. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS

R. H. Bragg
Phone: (415)-642-7393
$125,000 01-3

The relationship of the properties of hard carbons and soft carbons to their structure. Glassy carbon studied as a model hard carbon. Specific atomic mechanism(s) associated with the structural changes during graphitization.

155. HIGH-TEMPERATURE OXIDATION AND CORROSION OF MATERIALS

A. W. Searcy
Phone: (FTS) 451-6062 or (415)-486-6062
$350,000 01-3

A program to understand: a) the mechanisms by which materials withstand high-temperature corrosive attack, and b) the development of protective scales. Factors of major significance include: the initial development of the protective scale; the transport of reactants in and through the scale; the scales structure, morphology, and growth mode; the chemical integrity of the scale when exposed to corrosive sulfate deposits. The ultimate goal is to relate mechanisms of behavior to the thermodynamic, diffusional, structural, and compositional parameters of the metal oxides, sulfides, and other phases involved, and to develop both quantitative and predictive alloy corrosion models.

156. CERAMIC INTERFACES

A. M. Glaeser
Phone: (415)-642-3821
$125,000 01-3

Development of an improved understanding of processes that control microstructural changes during materials fabrication and utilization. Thermodynamic and kinetic models of the modifying effect of dihedral angle on the morphological stability of continuous grain boundary phases, e.g., continuous pore channels present during sintering and continuous second phases in eutectic alloys and composites. The effect of solute additions, specifically MgO, on the nature of grain boundary migration in pore-free Al_2O_3. Grain boundary migration in lead. Fabrication of oxide powders to study particle coarsening by vapor phase transport. The recrystallization behavior of cold-pressed, NaCl powder.

157. ABRASIVE, EROSIVE AND SLIDING WEAR OF MATERIALS

I. Finnie
Phone: (415)-642-1496
$120,000 01-5

Determination of the basic mechanisms of abrasive, erosive and sliding wear. Identification of similarities and differences in different types of wear to allow development of simpler screening tests. Examination of material properties and microstructural features needed for optimum wear resistance. Development of quantitative methods of wear prediction for both single phase and heterogeneous materials.

LAWRENCE BERKELEY LABORATORY (continued)

158. EROSION-CORROSION WEAR PROGRAM

A. W. Searcy
Phone: (FTS) 451-6062 or (415)-486-6062
$15,000 01-5

Development of a model for predicting erosion of ductile metals from analytical expressions that define the two-phase fluid flow of a gas-solid particle stream and equations that describe the platelet mechanism of erosion. Experimental studies of boundary layer gas to protect the surface of coal reactors from high-temperature corrosion.

159. EROSION OF BRITTLE SOLIDS

A. G. Evans
Phone: (415)-642-7347
$130,000 01-5

Development of a fundamental understanding of erosion and strength degradation of brittle coatings and layers subject to impact by solid particles. Studies of the damage created by individual particles and of the erosion characteristics under multiple impact conditions; consideration of residual stresses in the coatings and the adherence to the substrate. Predictions of material removal by spalling, after projectile impact.

160. FAR INFRARED SPECTROSCOPY

P. L. Richards
Phone: (415)-642-3207
$228,000 02-2

Development of improved types of infrared detectors, mixers, and spectrometers. Improved infrared techniques for experiments in areas of fundamental and applied infrared physics. Developments of infrared technology: a liquid helium cooled diffraction grating spectroscopy, fabrication and testing of ultrasensitive photoconductive detectors for the 50-500 µm wavelength range, improved fabrication for bolometric detectors with improved ultimate sensitivity, development of a new class of far infrared dichroic beam dividers, and development of far infrared harmonic generation as a spectroscopic source. Experiments in progress: measurements of the near infrared absorption spectra of molecules chemically adsorbed on metal surfaces, measurements of the infrared spectra of one-dimensional conductors including charge-density wave systems and organic superconductors, and measurements of the infrared photoconductivity of impurities in semiconductors.

LAWRENCE BERKELEY LABORATORY (continued)

161. EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS

Y. R. Shen
Phone: (415)-642-4856
$264,000 02-2

Emphasis is on development of linear and nonlinear laser and optical techniques for material studies and applications of these techniques to study linear and nonlinear optical properties of gases, liquids, liquid crystals, and solids. Both theoretical and experimental research on various aspects of light interaction with matter. Newly developed techniques used to study current problems of interest: isotope separation, photochemistry, surface physics, and phase transitions, and other nonlinear optical effects in matter.

162. EXCITATION IN SOLIDS

C. D. Jeffries
Phone: (415)-642-3382
$170,000 02-2

Studies of the onset of instabilities and pseudorandum behavior in solids, detailed analysis and interpretation within the recently developed renormalization group theory of chaotic dynamics, which displays universality and predicts that similar and recognizable modes of behavior will be observed in a very broad class of nonlinear phenomena, e.g., turbulence in fluids; plasma instabilities; erratic behavior in nonlinear mechanical, electrical and chemical systems; and various instabilities in semiconducting, magnetic, ferroelectric and piezoelectric materials. To facilitate direct comparison between observed behavior and theoretical models, development of specific experimental methods: bifurcation diagrams, phase space portraits, Poincare sections, return maps, power spectral analysis, real time and transient analysis, and probability density distributions. Concentration on spin waves in ferrities and on semiconductors. A detailed and systematic study of the chaotic dynamics of driven p-n junctions in Si and Ge revealed many universal patterns: periodic doubling bifurcations, onset of chaos, periodic windows, and intermittency. Spin wave instabilities in ferrite spheres display period doubling, chaos, and intermittency and understood by two-dimensional quadratic map. Electron-hole plasma density waves in crystals of Ge exhibit a period doubling route to chaos, periodic windows, and quasi-periodicity. Results bear on devices of high technological interest, and on a very general class of nonlinear problems of practical importance.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

163. TIME RESOLVED SPECTROSCOPIES IN SOLIDS

P. Y. Yu
Phone: (415)-642-8087

	$80,000	02-2

Use of fast picosecond tunable laser pulses produced by modelocked dye lasers, to study the processes associated with interactions between elementary excitations in condensed matter in real time to determine strength of these interactions. Current investigations involve: properties of dense electron-hole plasma created by picosecond laser pulses in semiconductors by light scattering spectroscopies and time-resolved emission spectroscopy; trapping of free carriers at deep, nonradiative centers in crystalline or disordered semiconductors; and carrier relaxation mechanisms in crystalline and amorphous solids.

164. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE

J. Clarke
Phone: (415)-642-3069

	$288,000	02-2

DC Superconducting QUantum Interference Devices (SQUIDs) developed and used in a wide variety of applications, including geophysical measurements, noise thermometry in the milliKelvin temperature range, nonequilibrium superconductivity, and the measurement of electrical noise. An ultra low noise SQUID amplifier operating at frequencies of up to 100 MHz used to improve the sensitivity of nuclear magnetic resonance and quadrupole resonance measurements. SQUIDs operating at temperatures down to 20 mK used to study their ultimate noise limitations for such applications as transducers for gravity wave antennas. Novel investigations of macroscopic quantum tunneling in Josephson tunnel junctions at millikelvin temperatures. The nonlinear dynamics of circuits containing a Josephson junction being studied, with particular regard to the noise in such systems. A detailed study of the excess noise induced in metal films by electron bombardment in an electron microscope. This type of measurement may provide a new technique for characterizing the defect concentration of metals.

165. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES

L. M. Falicov
Phone: (415)-642-5993
$75,000 02-3

A study of the properties of solid surfaces, in particular: (a) Structural properties of surfaces, namely the organization and arrangement of atomic constituents at equilibrium; (b) Constitutional properties of the surface, in particular the segregation properties of alloys at the surface as a function of crystal structure, surface orientation, nominal chemical composition and temperature; (c) Electronic structure of surfaces, electron states and electron densities in the neighborhood of the surface; (d) Vibronic properties of surfaces; (e) Magnetic properties of surface, both in magnetic solids (ferromagnetic and antiferromagnetic) or in nonmagnetic solids which may develop a magnetic surface layer; (f) Chemical catalytic properties of solids as they are related to basic physical properties (a)-(e). A variety of theoretical techniques and models to focus on the various properties (band-structure models, many-body body electron physics, numerical relaxation techniques) developed, but the emphasis is on physical aspects and their implication to experiments rather than techniques per se.

166. THEORETICAL SOLID STATE PHYSICS

M. L. Cohen
Phone: (415)-642-4753
$105,000 02-3

To provide a microscopic theory of solids capable of explaining and predicting the physical properties of real materials. A successful theory based on a quantum mechanical pseudopotential-local density-total energy approach with inputs essentially of only the atomic number and atomic mass of the constituent atoms making up a solid developed. Applications of the method to: surfaces, interfaces, optical properties, superconductivity, electronic structure, vibrational properties, static structural properties, high pressure solid phase transitions, transport, photoemission, chemisorption, and properties of molecules. Direct collaborations with experimental projects are frequent, and the predictive power of the approach has been tested successfully.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

167. LOW TEMPERATURE PROPERTIES OF MATERIALS

N. E. Phillips
Phone: (415)-642-4855

$130,000	03-1

Research on low temperature properties of materials and on methods of temperature measurement. Measurements on $_3$He in the Fermi-liquid region have established the correct values of parameters which are important to understanding superfluid states; on potassium, rubidium, and cesium to 0.1 K to test theoretical predictions of charge density wave effects; and on CuMn in high magnetic fields that have mapped out the theoretically predicted phase boundary of the spin-glass phase. Specific future objectives: an extension of the $_3$He measurements to the superfluid phases, additional studies on spin glasses, and specific heat measurements at pressures to 20 kbar on mixed-valence compounds.

168. ELECTROCHEMICAL PROCESSES

C. W. Tobias
Phone: (415)-642-3764

$120,000	03-1

Novel methods for reducing mass transfer resistance in high rate applications, e.g. effects of fixed flow obstacles and of suspended inert solid particles in flowing electrolytes. Nonaqueous ionizing solvents investigated for potential use in ambient temperature electrosynthesis processes. Techniques for the removal of trace impurities in propylene carbonate to below 10 ppb., to improve solvent stability in presence of energetic oxidizing- or reducing-agents.

169. HIGH-TEMPERATURE THERMODYNAMICS

L. Brewer
Phone: (415)-486-5946

$160,000	03-3

Development of models of predictive capability for the behavior of gases at high temperatures, of refractory containment materials, and of many metallic systems. The main thrust of the present research aimed at providing quantitative predictive models for the strongly interacting alloys exhibiting generalized Lewis acid-base behavior. A variety of experimental methods used to characterize the thermodynamics of these systems.

LAWRENCE BERKELEY LABORATORY (continued)

170. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES

D. R. Olander
Phone: (415)-642-7055

$275,000	03-3

To characterize the chemical and physical behavior of materials in the high temperature, radiation environment of fission and fusion reactors. The materials of the uranium-based fuels and the zirconium-based cladding materials of light-water nuclear reactors of principal interest. The processes and properties studied include rapid transient vaporization of fuel materials by laser pulsing, high temperature corrosion of zirconium by steam, and the release of volatile fission products from irradiated UO_2. Molecular beam studies of the chemical kinetics of gas-solid reactions, including hydrogen atom reactions with silicon and its compounds and the etching of metals of halogens.

171. PLASMA ENHANCED DEPOSITION OF THIN FILMS

D. W. Hess
Phone: (415)-642-4862

$20,000	03-3

Research on rf plasma enhanced deposition of thin films. Control of chemical, physical, and electrical properties by variation of deposition parameters. The final phase of this program.

LAWRENCE BERKELEY LABORATORY (continued)

172. ELECTROCHEMICAL PHASE BOUNDARIES

R. H. Muller
Phone: (FTS) 451-6079 or (415)-486-6079
$180,000 03-3

To advance the understanding of boundary layers and thin films at electrochemical interfaces. New optical techniques for the observation of electrode surfaces in liquid media developed and used: spectroscopic ellipsometry combined with light scattering measurement, Auger spectroscopy, interferometry, thin film interference, and Doppler velocimetry.

173. SOLID STATE AND SURFACE REACTIONS

G. A. Somorjai
Phone: (FTS) 451-6160 or (415)-486-6160; (415)-642-4053
$390,000 03-3

Studies of catalyzed surface reactions and investigations of the atomic structure of solid surfaces and adsorbed monolayers. The kinetics and mechanisms of catalytic surface reactions studied using well-characterized crystal surfaces at low and high pressures by using a combination of surface science techniques. Focus on platinum, rhodium, iron and its compounds, rhenium, molybdenum, alkali metals and bimetallic alloys. The adsorbates and reactants are mostly hydrocarbons, oxygen, hydrogen and water. Investigation directed toward an atomic scale understanding of the structure and catalytic behavior of metal surfaces, and at developing new catalysts which substitute for precious metals and exhibit high rates and selectivity.

174. NUCLEAR MAGNETIC RESONANCE

A. Pines
Phone: (FTS) 451-6097 or (415)-486-6097; (415)-642-1220
$195,000 03-3

Research on methods in magnetic resonance spectroscopy and study of molecular behavior in condensed phases. Novel methods developed include multiple quantum spectroscopy high resolution solid state NMR and magic angle spinning, zero field NMR, pulsed laser nuclear double resonance and nuclear magnetic isotope separation. These methods applied to determination of structure and dynamics at the molecular level in a number of materials including ferroelectrics, liquid crystals, polymers, organic crystals and zeolites. New methods of detection developed to increase the sensitivity of detection, in particular using rapidly switched superconducting fields and Josephson junction devices such as SQUIDS.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

Accelerator and Fusion Research Division - 02 -

175. R&D ON ADVANCED PHOTON SYSTEM

T. Elioff, R. Yourd, D. Attwood
Phone: (FTS) 451-4024 or (415)-485-4024
$2,200,000 02-2

Research and development of advanced accelerator systems and state-of-the-art components for high-brightness synchrotron beamlines and advanced insertion devices (wigglers and undulators). Associated research activities include the development of next-generation wigglers and undulators, of advanced beam line components and optical elements. Experimental facilities developed to match the needs of future experiments requiring high spectral brilliance. Accelerator Research includes the development of advanced computer control systems, precision instrumentation, radiofrequency systems with reduced higher order modes, a fast booster extraction system, ultra high vacuum systems and techniques, and studies to assure attainment of high current-low emittance electron beams for maximum spectral brilliance.

176. CENTER FOR X-RAY OPTICS (see also page D-27)

D. Attwood
Phone: (FTS) 451-4463 or (415)-486-4463
$1,000,000 02-2

Development of technologies required for the utilization of emerging sources of XUV radiation in application for science and industry. The Center has organized laboratories and collaborations which will lead to the development and broad utilization of new technologies for the production, efficient transport, focusing, dispersion and detection of radiation with photon energies extending from several eV to many keV. Development of coherent XUV radiation sources based on modern electron storage rings and the use of permanent magnet periodic structures. The activities of the Center have the common goal of extending the use of XUV radiation for basic and applied research.

177. CENTER FOR ADVANCED MATERIALS: CATALYSTS CERAMICS; ELECTRONIC MATERIALS; POLYMERS; INSTRUMENTATION FOR SURFACE SCIENCE

K. S. Pitzer, J. Clarke, L. C. De Jonghe, M. M. Denn, E. E. Haller,
G. A. Somorjai, A. G. Evans
Phone: (FTS) 451-4755 or (415)-486-4755
$2,300,000 01-1, 02-2, 03-3

Investigations of the mechanisms of defect formation and contamination during bulk crystal growth of gallium arsenide and other III-V semiconductors. Investigations of the relationship between the structure and electronic properties of semiconductor interfaces, and determination of the effects of substrate defects on the quality of epitaxial thin films. Synthesis and structural and catalytic characterization of heterogeneous catalysts: zeolites, transition metal compounds, and other novel catalytic materials. Investigations of the relationship between processing and microstructures of structural polymers and polymer composites focusing on polymer liquid crystals, short-fiber polymer composites, block copolymers, coprocessing of immiscible fluids, and interactions among polymers, solvents, and non-solvents. Development of advanced instrumentation (such as a tunneling microscope) for characterizing surfaces and interfaces that are important to high-technology or materials-based industries. Investigations to strengthen the scientific base needed for the development of advanced, high-temperature structural ceramics. Areas of study here include colloid behavior of powders, ceramic fabrication, high temperature mechanical properties of ceramics and evaluation of erosion and wear. Research on powder suspensions, sintering, crack nucleation and failure prediction is included.

LABORATORIES

LAWRENCE LIVERMORE NATIONAL LABORATORY
P. O. Box 808
Livermore, California 94550

Chemistry & Materials Science Department

R. M. Alire - Phone (FTS) 532-6340 or 415-422-6340

190. RAPID SOLIDIFICATION PROCESSING OF ALLOYS: STRUCTURE, PHASE RELATIONS AND PHASE TRANSFORMATIONS

L. Tanner, L. Jacobson
Phone: (FTS) 543-2653 or (415)-443-2653
$420,000 01-1

Preparation of rapidly quenched alloys based on aluminum with beryllium and lithium by arc-hammer splat, ribbon spinning and electron beam surface melting; characterization of microstructures produced at different solidification rates by optical and electron microscopy, high resolution TEM, and atom probe; determination of alloy response to thermal treatments by differential scanning calorimetry, differential thermal analysis and microstructure characterization; correlation of results with current thermodynamic kinetic models of solidification. Employ rapid solidification as a means of preparing alloys of Fe-Pd, Fe-Pt, Au-Ni, etc. in order to investigate phenomena associated with displacive phase transformations.

191. METASTABLE ALLOY SURFACES PRODUCED BY DIRECTED ENERGY LASER, ELECTRON AND ION BEAMS

E. N. Kaufmann
Phone: (FTS) 543-2640 or (415)-423-2640
$230,000 01-1

Investigations of microstructures produced in alloy layers created by rapid heating and cooling via electron- or laser-beams and by atomic mixing via ion-beams. Studies of the dependence of crystalline phase and glass formation as a function of binary phase relationships, epitaxial relationships, and resolidification velocity. Studies of the morphology of layers formed from film-on-substrate and bulk alloy starting geometries. Comparisons of laser- and electron-beam processing modes. Analysis using electron microscopy, optical microscopy, X-ray diffraction, Auger and Ion-Beam spectroscopies.

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

192. RAPID SOLIDIFICATION, COMPACTION, AND STRUCTURAL CHANGES BY DYNAMIC PRESSURE

W. J. Nellis, W. C. Moss, H. B. Radousky
Phone: (FTS) 532-7200 or (415)-432-7200
$100,000 01-1

Structures of materials induced by high dynamic pressure of ≤ 1 Mbar. Cause and effect relationship between the initial and final material states and the dynamic path that connects them. Structure and residual effects of dynamic pressure on the superconducting transition temperature of Nb and the magnetic properties of Fe. Variation of microstructure of anisotropic magnetic compounds by rapid quenching from high dynamic pressure, density and temperature and the effect on material strength and magnetization.

193. OPTICAL MATERIALS RESEARCH

N. Winter
Phone: (FTS) 532-6215 or (415)-422-6215
$470,000 02-2

New optical materials for high-power lasers prepared and characterized. Materials of interest include both transmitting optics and active media for solid-state lasers. Optical spectroscopy used to determine those properties affecting the energy storage and extraction capabilities of different laser ion-host combinations. Nonlinear optical properties of materials subject to intense light beams are also investigated. Studies of multiphoton absorption processes and intensity-dependent changes in refractive index. Measurements of optical and spectroscopic properties correlated with theoreticl calculations of local fields and electronic structure. State-of-the-art theoretical calculations of the optical properties of various ion-host combinations. The growth of new oxide and fluoride crystals for laser and nonlinear optics applications explored and measurements made of their physical and chemical properties.

194. SURFACE PHYSICS AND CHEMISTRY OF LASER-INDUCED DAMAGE

W. J. Siekhaus
Phone: (FTS) 532-6884 or (415)-432-6884
$300,000 02-2

Investigation of physical and chemical mechanisms leading to laser surface systems. Experiments measuring with high spatial resolution multiphoton electron emission from semiconductor and insulator surfaces. Spacially resolved time of flight mass spectrometric studies of laser induced ion emission resulting in laser surface damage.

LABORATORIES

LOS ALAMOS NATIONAL LABORATORY
P. O. Box 1663
Los Alamos, New Mexico 87545

Materials Science and Technology Division - 01, 03

S. S. Hecker - Phone (FTS) 843-4563 or 505-667-4563

200. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF CERAMIC NUCLEAR WASTE

F. W. Clinard Jr.
Phone: (505)-667-5102

$310,000 01-4

Alpha decay self-damage in zirconolite, perovskite, pyrochlore, and multiphase SYNROC ceramic waste. Doping with short half-life actinides and examination of natural mineral analogues. Role of starting composition and crystal structure. Evolution of the metamict state; localized and generalized atomic disorder; alpha recoil tracks. Simulation of damage by ion irradiation. Characterization of damage effects by x-ray and electron diffraction, optical and electron microscopy, EXAFS, dilatometry, calorimetry, and fractography. Changes in density (swelling), microhardness, fracture toughness, and resistance to microcracking. Effect of elevated temperature during self-damage; post-irradiation annealing and recovery.

201. MECHANICAL PROPERTIES

M. G. Stout, N. F. Kochs, P. Follansbee, P. Martin
Phone: (505)-667-6750

$590,000 01-5

Response of metals to multiaxial loading and large strains; yield surfaces, multiaxial stress-strain relationships, stress path changes. Characteristics of and mechanisms controlling the large strain deformation of aluminum, nickel, copper, brass; substructural and textural evolution with strain and strain state. Multi-axial loading brittle fracture responses of Al_2O_3, Si_3N_4, SiC and ZrO_2; Statistical fracture theories for mixed-mode fracture of indention-produced surface flaws and macroscopic cracks; microstructural effects on multiaxial loading brittle fracture.

LOS ALAMOS NATIONAL LABORATORY (continued)

202. STRUCTURAL CERAMICS

J. J. Petrovic, D. S. Phillips
Phone: (505)-667-5913
$290,000 01-5

Fabrication-microstructure-properties interrelationships for structural ceramic materials; synthesis of dense, strong SiC and Si_3N_4 without the use of densification additives that can degrade elevated temperature mechanical properties and affect property reproducibility; RF-plasma synthesis of ultra-fine/ultra-pure SiC and Si_3N_4 powders; powder activation to enhance densification, using explosive shock loading and ion irradiation treatments; colloidal chemistry approaches to the synthesis of high green density bodies with uniform porosity distribution; dependencies of properties on processing and microstructure.

203. IMPURITY MODIFICATION OF MATERIALS: SURFACE PROPERTIES AND THIN STRUCTURAL FILMS

T. N. Taylor
Phone: (505)-667-7712
$240,000 03-2

Selective modification of chemisorption properties by surface additives. Relationship that electronic, structural, and compositional factors have to surface reactivity. Study of vapor deposited metal and semimetal adatoms on single-crystal desorption spectroscopies, low-energy electron diffraction and work function measurements. Crystallographic characterization by MeV ion scattering. Structural and mechanical properties of vapor deposited thin film metal/metal-compound laminates. Spatial and chemical nature of impurity layers by energetic ion beam analysis and conventional surface sensitive techniques. Physical and mechanical properties of vapor deposited films.

LOS ALAMOS NATIONAL LABORATORY (continued)

Physics Division - 02 -

J. C. Browne - Phone (FTS) 843-6162 or 505-667-6162

204. CONDENSED MATTER RESEARCH WITH THE SNR/PSR FACILITY (see also page D-9)

R. N. Silver
Phone: (505)-667-6069
$1,570,000 02-1

Neutron scattering research in condensed matter using the SNR/PSR pulsed spallation neutron source at Los Alamos. Studies in most areas of condensed matter; currently metal hydrides, catalysts, liquids, metallic glasses, magnetism, chemical structure, chemical spectroscopy, etc. The SNR/PSR is a national user facility for neutron scattering research in solid state physics, chemistry, materials science, biology, and polymers with the following time-of-flight spectrometers currently in the user program: single-crystal diffractometer, filter difference spectrometer and a powder diffractometer.

205. ULTRAHIGH-PRESSURE STUDIES OF MOLECULAR CRYSTALS

R. L. Mills
Phone: (505)-667-4129
$220,000 02-2

Studies of solidification, crystal structures, phase transformations, and thermodynamics of simple dielectrics, hydrides, and polymers from low to high temperature in high-pressure diamond anvil cells (DACs) using UV, IR, and Raman spectroscopy and laser-beam, neutron, and X-ray scattering; develop theories of phase transformation, structural behavior, and chemical reaction kinetics; use DACs to prepare and characterize exotic materials, including rare-gas and hydrogen-containing molecules.

206. THERMAL PHYSICS

J. C. Wheatley
Phone: (505)-667-7499
$250,000 02-2

Natural or intrinsically irreversible engines: acoustic engines using liquids and gases, magnetic engines, heat pumps and prime movers; liquid propylene thermodynamic and thermophysical properties; liquid propylene heat engine: regenerators, heat exchangers, mechanicals, seals; thermal convection in dilute solutions of ^{3}He is superfluid ^{4}He near 1 K, steady and oscillatory, nonlinear dynamics, coherence and chaos; spin polarized hydrogen isotopes: transport, thermodynamic properties, magnetosound; normal and superfluid liquid ^{3}He: ferromagnetism, susceptibility anisotropy.

LABORATORIES

LOS ALAMOS NATIONAL LABORATORY (continued)

Theoretical Division - 01, 02

G. I. Bell - Phone: (FTS) 843-4401 or 505-667-4401

207. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW AND MICROSTRUCTURE CHARACTERIZATION

J. E. Gubernatis
Phone: (505)-667-6727
$180,000 01-5

Development of an analytical scientific reference data base for flaw and microstructure characterization calculations of phenomena selected as representative of applications; integral equation methods, the method of optimized truncation, geometrical diffraction theory and Pade approximations; single scattering results for the flaw characterization studies; multiple scattering theories for the microstructure characterization studies. Investigate use of elastic wave scattering measurements for residual stress evaluation and for characterization of surface cracks.

208. LOS ALAMOS EQUATION OF STATE LIBRARY

J. D. Johnson
Phone: (505)-667-4053
$250,000 02-3

A computer-based library of equations of state (EOS) and other material properties such as opacities, and electrical and thermal conductivities for application to energy and related programs. Survey current user requirements and calculate or acquire and evaluate the needed data Data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Library programs and data available to users on magnetic tapes in a universal computer format. Theories of solids, liquids, gases, plasmas, and mixtures used to generation of EOS data. Development of new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY
P. O. Box X
Oak Ridge, Tennessee 37831

Metals and Ceramics Division - 01 -

J. R. Weir, Jr. - Phone (FTS) 624-4065 or 615-574-4065
C. J. McHargue - Phone (FTS) 624-4344 or 615-574-4344

215. THEORETICAL STUDIES OF METALS AND ALLOYS

J. S. Faulkner, W. H. Butler, G. S. Painter, G. M. Stocks,
D. M. Nicholson
Phone: (615)-574-5161
$632,000 01-1

The KKR-CPA method for calculating the electronic states of alloys provides the basis for explaining experiments on alloy systems such as photoemission, positron annihilation, soft X-ray emission and absorption, resistivity, low-temperature specific heats, etc. The high-speed band theory technique QKKR is used to calculate total energies of metals and intermetallic compounds. Results are coupled with KKR-CPA calculations to obtain insights into the thermodynamic parameters that determine the phase stability of alloy systems. The KKR-CPA method is used to study magnetism at finite temperatures, and order in alloys. Electron-phonon interactions are calculated and used to explain resistivities of normal metals and superconductors. Cluster and layer techniques are used to calculate the physical and chemical properties of surfaces interacting with their environment. Studies of metal-metalloid clusters are applied to grain-boundary segregation and cohesion.

216. X-RAY RESEARCH USING SYNCHROTRON RADIATION

C. J. Sparks, B. S. Borie, G. E. Ice, H. L. Yakel
Phone: (615)-574-6996
$639,000 01-1

Development and use of flourescence, anomalous dispersion, and scattering techniques for X-rays at the Stanford Synchrotron Radiation Laboratory; design and construction of beam line for installation at the National Synchrotron Light Source, Brookhaven National Laboratory; long- and/or short-range order in Fe-Ni-Cr alloys; atom positions in sigma phase, and alloyed carbides; defects in ion implanted materials; theoretical studies of extinction phenomena.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

217. MICROSCOPY AND MICROANALYSIS

J. Bentley, E. A. Kenik, M. K. Miller, P. S. Sklad
Phone: (615)-574-5067
$432,000 01-1

Development and application of analytical transmission microscopy and HVEM to determine the microstructure and microchemistry of solids; weakbeam darkfield studies of precipitates in irradiated alloys; lattice imaging of two-phase interfaces; SAES and EELS of internally oxidized refractory metal alloys; structure of long-range ordered alloys; in situ deformation, oxidation, and hydriding studies in the 1-MeV microscope; grain boundary phases in structrural ceramics; structure of metallic glasses; standardless EELS analysis; development of Imaging Atom Probe.

218. DEFORMATION AND FRACTURE OF METALS AND ALLOYS

M. H. Yoo, J. Schneibel, C. L. White, G. F. Petersen
Phone: (615)-574-5165
$498,000 01-2

Experimental and theoretical studies of effects of impurities and interfaces on deformation and fracture of Ni, Fe-Ni, Ni-Cr, Fe-Ni-Cr, and Ni_3Al alloys; grain boundary cavity nucleation and growth; segregation of impurities to grain boundaries and creep cativities; dynamic recrystallization; small-angle neutron scattering studies of cavity growth during creep and fatigue in nickel and austenitic stainless steel.

219. MECHANICAL PROPERTIES OF CERAMICS

P. F. Becher, M. K. Ferber, C. S. Yust, P. Angelini
Phone: (615)-574-5157
$539,000 01-2

Toughening behavior and slow crack growth mechanisms in polycrystalline TiB_2 as related to internal stress, microcracking, and microstructure; wear studies of TiB_2, SiC, Al_2O_3, and transformation-toughened Al_2O_3-Zr_2O_3; slow crack growth and toughening behavior in transformation-toughened Al_2O_3-Zr_2O_3, dispersion-toughened SiC.

220. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS

J. V. Cathcart, R. E. Druschel, R. A. McKee, R. E. Pawel
Phone: (615)-574-4925
$533,000 01-3

Reaction kinetics and defect interactions during diffusion in growing sulfide scales; high temperature oxidation of Ni_3Al-base alloys; diffusion in doped FeS crystals; oxide scale adherence studies; dynamic resonance measurements of elastic and anelastic properties of scales; theoretical treatment of diffusion in highly defective oxides.

221. METASTABLE MATERIALS

D. M. Kroeger, D. S. Easton, J. A. Horton
Phone: (615)-574-5156
$530,000 01-3

Relationships among composition, structure, and physical properties of metallic glasses; glass stability; effects of impurity additions on structure and properties of metallic glasses; preparation techniques by arc-hammer, melt-spinning and electron-beam vapor deposition; mechanical properties; low temperature specific heat; small-angle scattering and TEM studies of defect structure, and phase separation in metallic glasses.

222. RADIATION EFFECTS

L. K. Mansur, R. E. Clausing, K. Farrell, L. L. Horton, E. H. Lee, M. B. Lewis, N. H. Packan
Phone: (615)-574-4797
$1,540,000 01-4

Mechanisms of radiation effects; neutron damage in pure metals, alloys, and ceramics irradiated in ORR, HFIR, and EBR-II, effect of alloying additions, impurities and microstructure on void nucleation and growth; phase stability under irradiation; ion irradiation studies using multiple ion beams (heavy and dual light ions), relationship between ion and neutron damage, effect of helium and other gases on nucleation and growth of voids and interstitial loops; theory of void and loop nucleation and growth, solute-defect interactions, irradiation creep, cascade diffusion theory; Fe, Al, Zr, Ni, and alloys, stainless steels, ferritic alloys, ceramics.

223. FUNDAMENTALS OF WELDING AND JOINING

S. A. David, J. M. Vitek
Phone: (615)-574-4804
$444,000 01-5

Control of weld microstructure through control of solidification parameters; composition, distribution, and stability of microphases; microstructure of laser-produced welds; hot cracking; modeling of solidification processes; structure-property correlations, austenitic and ferritic stainless steels, electron beam welding, American Welding Technology Application Center (AWTAC) Projects.

OAK RIDGE NATIONAL LABORATORY (continued)

224. HIGH TEMPERATURE ALLOY DESIGN

C. T. Liu, J. A. Horton, A. DasGupta, W. C. Oliver
Phone: (615)-574-4459

\$344,000	01-5

Design of ductile polycrystal alloys based on Ni_3Al; microalloying with B; macroalloying with Fe, Hf, Ce; creep, oxidation and physical properties; structure and composition of grain boundaries, nature and effects of defects.

225. RESEARCH IN CERAMIC PROCESSING

P. F. Becher, C. B. Finch, P. Angelini, A. Bleier, S. Baik
Phone: (615)-574-5157

\$399,000	01-5

Sintering behavior of TiB_2 including liquid phase effects, the role of oxygen and carbon; AEM characterization of second phase formation, crystal growth and characterization of properties of boride phases; synthesis of ZrO_2 and Al_2O_3 powders and effects of powder surface characteristics on densification in transformation-toughened Al_2O_3-ZrO_2 type composites; AEM studies on alloying and microstructural effects in transformation behavior.

226. ION BEAM PROCESSING OF MATERIALS

C. J. McHargue, P. S. Sklad, C. S. Yust, M. B. Lewis
Phone: (615)-574-4344

\$250,000	01-5

Structure of ion-implanted Al_2O_3, SiC, and TiB_2 by backscattering-channeling and TEM, hardening, surface fracture toughening and wear of ion-implanted ceramics, structure and properties studied as a function of implantation parameters (temperature, fluence, energy, ion species) and annealing (temperature and environment).

OAK RIDGE NATIONAL LABORATORY (continued)

Solid State Division - 02 -

M. K. Wilkinson - Phone (FTS) 624-6151 or 615-574-6151
F. W. Young, Jr. - Phone (FTS) 624-5501 or 615-574-5501

227. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS

R. M. Nicklow, J. R. Arthur, J. W. Cable, H. R. Child, S. Funahashi, J. B. Hayter, S. Kawarazaki, W. C. Koehler, J. W. Lynn, H. A. Mook, R. M. Moon, O. A. Pringle, H. G. Smith, Y. Tsunoda
Phone: (615)-574-5240
$1,080,000 02-1

Inelastic neutron scattering studies of phonons, magnons, and single-particle excitations in condensed matter; elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials; lattice dynamics of α-Ce, SmB_6, Ba, and intercalated graphite; magnetic excitations in Cu(Mn), amorphous materials, paramagnetic Ni and Fe, and Gd; phase transitions in In(Tl) alloys, Ni_3Mn, Cu_3Au, and random field systems; magnetic form factors of mixed-valence materials; structures of composition modulated systems and nuclear spin ordering.

228. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES

J. W. Cable, J. R. Arthur, H. R. Child, S. Funahashi, M. Iizumi, S. Katano, W. C. Koehler, H. A. Mook, R. M. Moon, R. M. Nicklow, O. A. Pringle, H. G. Smith, S. Spooner, G. D. Wignall
Phone: (615)-574-5233
$770,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals; lattice dynamics of A15 com-pounds, $PdTe_2$, Fe(Cr) alloys, and KCl(CN); proton diffusion in biological systems and microemulsions; magnetic structures in GdD_2 and reentrant superconductors; SANS from coal solutions, oil shale, surfactants, metal alloys, and polymer blends; kinetics of spinodal decomposition.

229. SUPPORT FOR NEUTRON USERS' PROGRAM (see also page D-5)

H. A. Mook, J. W. Cable, H. R. Child, R. M. Moon, R. M. Nicklow, O. A. Pringle, H. G. Smith
Phone: (615)-574-5242
$320,000 02-1

ORNL neutron scattering facilities available to outside scientists through Neutron Users' Program; recent investigations include lattice dynamics of intercalated graphite, structure and dynamics of spin glasses, random field systems, polarized-beam studies of paramagnetism, metallic superlattices, proton diffusion in biological systems, and collagen periodicity in bones.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

230. PHYSICAL PROPERTIES OF SUPERCONDUCTORS

S. T. Sekula, Y. K. Chang, D. K. Christen, J. R. Ellis,
H. R. Kerchner, D. H. Lowndes, J. R. Thompson
Phone: (615)-574-6271
$415,000 02-2

Investigations of flux-line-lattice arrays, flux flow, flux creep, flux-line defect interactions, and anisotropy in refractory metal alloys and compounds with A15 and B1 crystal structures; small-angle neutron scattering by fluxline lattices in equilibrium and metastable configurations, dc magnetization, ac magnetic permeability, critical-current and normal-state electrical transport; ion damage and implantation in foil and thin film superconductors; low-temperature laser quenching of superconductors.

231. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION

R. F. Wood, R. B. James, E. Fogarassy, G. E. Jellison,
D. H. Lowndes, F. A. Modine, R. Ruckteschler, R. D. Westbrook,
R. T. Young
Phone: (615)-574-5781
$845,000 02-2

Time-resolved optical and electrical measurements of laser-induced melting and recrystallization; picosecond laser spectroscopy, laser-induced photochemical deposition; thermal and laser annealing of lattice damage in Si and GaAs; laser-induced recrystallization of amorphous layers; fabrication of high-efficiency Si solar cells by laser techniques; effects of point defects, defect clusters, dislocations, stacking faults, and chemical impurities on electrical and optical properties of single-crystal and polycrystalline Si; electrical, optical (including infrared and luminescence spectroscopy), transmission electron microscopy, X-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering property measurements; dopant concentration profiles, deep-level transient spectroscopy, and absolute quantum efficiency measurements; fabrication of test solar cells; solar cell modeling; thin-film deposition on prepared substrates; chemical vapor deposition of Si on low-cost substrates.

232. FUNDAMENTAL ASPECTS OF METAL FRACTURE

S. M. Ohr, S.-J. Chang, T. S. Noggle, C. G. Park
Phone: (615)-574-5509
$485,000 02-2

Experimental and theoretical investigations to relate phenomena of continuum fracture mechanics to microscopic physical phenomena occurring at a crack tip; in situ transmission electron microscope observations of crack propagation in aluminum, copper, nickel, molybdenum, niobium, tungsten, stainless steel, magnesium oxide, and niobium oxide; crack propagation in metals containing helium bubbles; distribution of dislocations in the plastic zone ahead of crack tip in metals and ceramics; cyclic deformation; ductile-brittle transition in bcc metals; dislocation theory of J-integral; theory of plastic zone with a dislocation-free zone; in situ TEM studies of crack propagation in gaseous (hydrogen) environment.

233. PHYSICAL PROPERTIES OF CERAMICS

F. A. Modine, C. Y. Allison, Y. Chen, G. R. Gruzalski,
J. R. Martinelli, E. Sonder, R. A. Weeks
Phone: (615)-574-6287
$685,000 02-2

Transition-metal carbides and nitrides and the refractory oxides; physical properties of materials characterized with regard to composition, defect structures, and phase segregation; studies involving charge and mass transport with emphasis on varistor materials, degradation, and high-temperature effects; techniques include optical and paramagnetic resonance spectroscopies, electrical properties measurements, and laser heating.

234. CHARGE TRANSPORT IN SOLID ELECTROLYTES

J. B. Bates, W. E. Brundage, Y. T. Chu, N. J. Dudney, J. C. Wang
Phone: (615)-574-6280
$405,000 02-2

Kinetics and thermodynamics of the hydration reaction of beta- and beta"-aluminas; effect of intercalated water on electrical properties; composite electrolytes and the mechanisms of ionic transport in multiphase materials; charge and mass transport at metal-dielectric and dielectric-dielectric interfaces; techniques include impedance spectroscopy, transient signal analysis, Raman scattering, infrared absorption, ATR and internal reflection spectroscopy, and electron microscopy; experimental results are interpreted and correlated by means of model calculations.

OAK RIDGE NATIONAL LABORATORY (continued)

235. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS

L. A. Boatner, M. M. Abraham, W. E. Brundage, Y. K. Chang
Phone: (615)-574-5492
$650,000 02-2

Development of new techniques for growth of single-crystal research specimens and for advanced materials preparation; techniques for the growth of single crystals with specified geometries; flux growth of single crystals of fast-ion conductors (beta-alumina, beta"-alumina); Czochralski and float-zone growth of crystals of Fe-Ni-Cr alloys (i.e., stainless steels); growth of refractory metal crystals (Ti, V, Zr, Nb, Ta, W, Ir, Re) using electron-beam float-zone technique; rf induction float-zone growth of transition-metal carbides; growth of perovskite-structure oxides ($KTaO_3$, $KTa_{1-x}Nb_xO_3$, CaTiO3) and semiconducting oxides for photoelectrochemical cell electrodes; float-zone and tri-arc growth of crystals of A15 compounds such as V_3Si, V_3Ge, and Ti_3Pt; arc-fusion and flux growth of crystals of high-temperature materials (WC, Y_2O_3, MgO, CaO, SrO); characterization of high-quality single crystals of metals, alloys, and insulators.

236. SMALL-ANGLE X-RAY SCATTERING (see also page D-11)

W. C. Koehler, J. S. Lin, S. Spooner
Phone: (615)-574-5232
$155,000 02-2

Small-angle X-ray scattering of metals, metallic glasses, precipitates, alloys, polymers, and surfactants; void distributions in oil shale and irradiated metals; dynamic deformation studies of polymers; time-slicing studies of phase transformations. Facilities are available to users through National Center for Small-Angle Scattering Research (NCSASR).

237. THEORY OF CONDENSED MATTER

J. F. Cooke, J. H. Barrett, H. L. Davis, R. J. Elliott, L. J. Gray, T. Kaplan, S. H. Liu, M. E. Mostoller, O. S. Oen, A. K. Rajagopal, M. Rasolt, M. T. Robinson, J. C. Wang, R. F. Wood
Phone: (615)-574-5787
$1,160,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors; superionic conductivity and solid electrolytes; lattice dynamics and potential energy calculations of ionic crystals; computer simulation of radiation damage and sputtering; radiation damage analysis procedures; radiation emitted by channeled electrons; reflection of light atoms from surfaces; surface studies with backscattered ions; development of LEED theory and interpretation of LEED data; surface vibrations and relaxation; correlation contributions to surface energy; optical potential for electron spectroscopies; theory of angular effects in photoemission and Auger emission of electrons from surface regions; electron screening; electronic structure of metal surfaces; lattice dynamics of transition metals; magnetism in transition metals; Brillouin zone integration; Heisenberg spin systems; metal-hydrogen interactions; high-temperature oxides and carbides; lattice vibrations in alloys; coherent potential approximation; neutron scattering from crystals, molecular-like impurities in crystals, and alloys; electronic properties of rare-earth and actinide compounds; band structure calculations for metals and insulators; electronic properties of mixed-valent systems; critical phenomena and phase transitions; dynamical properties of fractal systems.

238. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY

B. C. Larson, J. Narayan, D. Fathy, J. D. Lewis, T. S. Noggle, S. M. Ohr, C. G. Park, S. Pennycook, J. Z. Tischler
Phone: (615)-574-5506/5508
$850,000 02-4

Structure of intrinsic and induced defects in solids; transmission electron microscopy; synchrotron X-ray scattering; X-ray diffuse scattering; X-ray topography; defect clusters resulting from fast neutron and ion irradiations of metals; pulsed-laser annealing; defects associated with laser and thermal processing of pure and ion-implanted semiconductors; cell structure in doped semiconductors; grain boundaries in semiconductors; high-resolution atomic imaging of defects; structure of displacement cascades in silicon; solid-phase recrystallization in semiconductors; structure of high-temperature metal carbides; defects in high-temperature oxides; anisotropic elastic theory of dislocation loops; computer simulation of electron microscopy images; novel analytical techniques of electron microscopy; calculation of diffuse scattering from dislocation loops and solute precipitates; energy-resolved X-ray scattering; quasi-elastic scattering; phase transformations; theory of interactions of electrons and X-rays with defects in solids.

OAK RIDGE NATIONAL LABORATORY (continued)

239. SYNTHESIS AND PROPERTIES OF ISOTOPIC SOLIDS

L. A. Boatner, M. M. Abraham, J. O. Ramey, B. C. Sales
Phone: (615)-574-5492
$400,000 02-4

Application of enriched isotopes to the development of new advanced materials; tailoring of materials properties by means of stable and radioactive isotopes; production of isotopically enriched materials for detailed spectroscopic and materials characterization; use of isotopic solids in investigations of polycrystalline ceramics, glasses, single-crystal metals, and dielectrics; studies of physical, chemical, and mechanical properties of isotopic solids by means of optical absorption, electron paramagnetic resonance, Raman scattering, Mossbauer spectroscopy, ion implantation, Rutherford backscattering, and thermal analysis; exploitation of isotopic properties in resolving basic scientific problems; use of isotopes in the development of materials for applications in advanced materials-related technologies.

240. ESTABLISHMENT AND RESEARCH USE OF A NATIONAL LOW-TEMPERATURE IRRADIATION FACILITY

R. R. Coltman Jr., C. E. Klabunde
Phone: (615)-574-6263
$190,000 02-4

Design, construct, test, and operate for users a National Low-Temperature Neutron Irradiation Facility (NLTNIF) at the ORNL Bulk Shielding Reactor (BSR); determine neutronics characteristics in the irradiation cryostat for use at an in-core position and with several radiation modifying devices; provide data acquisition and computer equipment for users; design and construct specialized cryogenic test equipment; provide equipment and procedures for the transfer of irradiated specimens at 4.2 K.

241. SURFACE PHYSICS AND CATALYSIS

L. H. Jenkins, H. L. Davis, W. Erly, J. R. Noonan, G.-C. Wang,
J. F. Wendelken, C. W. White, D. M. Zehner
Phone: (615)-574-7031
$960,000 02-5

Studies of crystallographic and electronic structure of clean and adsorbate-covered metal binary alloy and semiconductor surfaces with emphasis on surfaces which either reconstruct or have interplanar spacings different from those of the bulk; combined techniques of low-energy electron diffraction (LEED), positive ion crystallography of surfaces (PICS), photoelectron spectroscopy (PES) using synchrotron radiation, and computer simulations for surface crystallography studies; LEED, PES, and Auger electron spectroscopy (AES) combined with in situ laser annealing of semiconductors; lineshape analysis of Auger spectra; LEED, AES and x-ray photoelectron spectroscopy (XPS) studies of both clean and adsorbate-covered surfaces of metals and intermetallic compounds; determination of effects of intrinsic and extrinsic surface defects on surface properties using LEED; vibronic structure of adsorbates examined by high-resolution electron energy loss spectroscopy (EELS); examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

242. SURFACE MODIFICATION AND CHARACTERIZATION (SMAC) FACILITY AND COLLABORATIVE RESEARCH CENTER (see also page D-21)

B. R. Appleton, O. E. Schow III, T. P. Sjoreen, C. W. White
Phone: (615)-574-6283
$500,000 02-5

SMAC facility for alteration of materials properties in UHV by ion implantation doping, pulsed-laser processing, and ion beam mixing at sample temperatures from 4-1300 K; in situ materials characterization by ion-beam analysis, ion channeling, electrical measurements, and surface analysis techniques; SMAC facility supports research in the Ion Beam Analysis and Ion Implantation Program and other ORNL divisions; SMAC facility is available to scientists outside ORNL for collaborative research projects through the SMAC Collaborative Research Center.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

243. ION BEAM ANALYSIS AND ION IMPLANTATION

B. R. Appleton, C. W. White, M. J. Aziz, J. H. Barrett,
G. M. Beardsley, R. J. Culbertson, G. C. Farlow, E. Fogarassy,
O. W. Holland, E. Kelly, O. E. Schow, J. M. Williams, S. P. Withrow
Phone: (615)-574-6283
$970,000 02-5

Fundamental studies of ion implantation damage and annealing; dynamic annealing during implantation; formation of buried amorphous or insulating layers by implantation; fundamental studies of ion beam mixing; positive ion crystallography of surfaces (PICS); ion-solid interactions (particulary ion channeling); pulsed-laser annealing and rapid solidification; high-speed nonequilibrium crystal growth; investigations of segregation, constitutional supercooling, solute trapping, and precipitate formation; mechanisms limiting maximum substitutional concentrations during rapid solidification; supersaturated substitutional alloys; new metastable phases and amorphous alloys fabricated by ion beam and pulsed-laser processing; rapid thermal annealing; solid-phase epitaxial regrowth; applications of ion implantation doping and pulsed-laser processing to studies of corrosion/catalysis mechanisms, to reduction of friction and wear of metal surfaces, to improvements in hardness and fracture toughness of ceramics, to improvements in high-temperature materials, and to superconducting materials fabrication; ion beam and pulsed-laser mixing in metals, semiconductors, and insulating substrates; ion implantation of surgical alloys; surface smoothing of laser mirrors.

244. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION

H. L. Adair, W. S. Aaron, M. Petek, T. C. Quinby, D. W. Ramey
Phone: (FTS) 574-5900
$340,000 02-5

Research and development of preparative techniques applicable to isotopic materials. Stable and radioactive isotopes prepared in the form of ultra-thin films (supported and self-supported), coatings, wires, rods, cast shapes, alloys, compounds, ceramics, cermets, and distilled metals; techniques of preparation include vapor deposition, sputtering (rf, dc, planar magnetron, and ion beam), rolling, electrodeposition, molecular plating, liquid phase and conventional sintering, hot pressing, reactive and conventional spray calcination, nonconsumable arc melting, vacuum distillation, conversion of organic precursors to oxide films and solid forms, He implantation in metals, and general inorganic chemical processing. In-house characterization methods include X-ray diffraction and fluorescence, metallographic and ceramographic sample preparation, optical microscopy, scanning electron microscopy with energy dispersion X-ray spectrometry, differential thermal analysis, microgravimetric determinations, thermal conductivity determinations, in-situ film thickness monitoring, and sophisticated radiation counting methods.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

Chemistry Division - 03 -

M. L. Poutsma - Phone (FTS) 624-5028 or 615-574-5028

245. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS

W. R. Busing, B. K. Annis, G. M. Brown, E. Johnson, A. H. Narten,
D. W. Noid, W. E. Thiessen
Phone: (FTS) 624-4976 or (615)-574-4976
$850,000 03-1

Atomic and molecular arrangements in crystals and in liquids determined by neutron and X-ray diffraction studies; atom-atom pair correlation functions for liquids; precise electron densities in crystals; neutron spectroscopy; development of synchrotron radiation facilities. Computational methods for dynamic correction of neutron scattering intensities; improvement of statistical mechanics techniques for application to ionic solutions or molten salts; use of computational models to interpret the effects of intermolecular packing forces on the geometry of molecules in crystals; calculation of physical properties of crystals. Materials studied include amorphous metal alloys, compounds which are potential catalysts for hydrogenation and hydrogen production, molten salts, aqueous lanthanide and actinide solutions, and silicate minerals of the earth's mantle.

246. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS

C. E. Bamberger, J. Brynestad, G. M. Begun, L. Maya
Phone: (FTS) 624-4944 or (615)-574-4944
$678,000 03-2

Synthesis of high-purity structural ceramic compounds by novel reactions; heterogeneous (gas-solid) reactions that yield extremely fine powders; reactions of titanium and titanium chlorides with gaseous BCl_3 to yield TiB_2 powder with particles size of 100 nm or less; chemistry of precursors formed at low temperatures; electrochemistry of aluminum in liquid ammonia; reactions of gaseous HF with commercial SiC to remove oxide contamination; reaction thermodynamics and mechanisms; compaction and sintering studies.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY

Chemical Technology Division - 03 -

R. G. Wymer - Phone (FTS) 624-6275 or 615-574-6275

247. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES

F. A. Posey, A. L. Bacarella, H. R. Bronstein, Gilbert M. Brown,
E. J. Kelly, C. E. Vallet
Phone: (FTS) 624-5022 or (615)-574-5022
$730,000 03-3

Mechanism of the hydorgen evolution reaction on titanium; theoretical and experimental studies on initiation and propagation of crevice corroison of titanium; autopassivation of titanium in localized corrosion; hydrolysis, speciation, and other medium effects on interfacial reaction kinetics in concentrated aqueous electrolytes encountered in localized corrosion; application of photoacoustic spectroscopy coupled with electrochemical measurements to in situ corrosion studies (film formation and breakdown, surface concentration and identity of reaction intermediates, etc.); theory of response of occluded corrosion systems to impedance and transient measurements.

248. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY-RELATED MATERIALS

T. B. Lindemer, T. M. Besmann, C. A. Culpepper
Phone: (FTS) 624-6275 or (615)-574-6850
$360,000 03-2

This program is designed to measure and interpret the chemical thermodynamic properties of the extensive solid solutions present in the U-Pu-RE-O systems, where RE represents the lanthanides. The thermodynamic properties of the actinide oxides are being studied experimentally and theoretically, as are general mathematical theories for determining chemical equilibrium in multicomponent systems. Much of this work is generally applicable to the prediction of the properties of nonstoichiometric oxide solid solutions and of multicomponent chemical systems.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

249. CHEMICAL ENGINEERING RESEARCH

C. H. Byers, D. F. Williams
Phone: (615)-574-4653

$302,000 03-2

Fundamental laser scattering measurements and theoretical framework for material transport and thermodynamic properties of liquid mixtures at high temperatures and pressures, often in the critical region. Methods development (including optical measurements, dispersion stabilization, and mathematical analysis) for properties measurement of organic mixtures such as those important in critical extraction and those found in coal conversion streams. Viscosities, diffusivities, and vapor-liquid equilibrium at high pressures and temperatures. Crystallization and growth of monodispersed seed materials, particle size analysis.

LABORATORIES

PACIFIC NORTHWEST LABORATORY
P. O. Box 999
Richland, Washington 99352

Materials Science Division - 01 -

S. D. Dahlgren - Phone (FTS) 444-0120 or 509-376-0120

260. HIGH TEMPERATURE CORROSION AND ELECTROCHEMICAL INTERACTIONS IN CERAMICS

J. L. Bates, D. D. Marchant
Phone: (509)-375-2579 or (509)-375-2997
$265,000 01-1

Mechanisms and kinetics of high-temperature reactions for refractory metal oxides with molten silicates, molten salts and gases. Dissolution of oxides, such as $MgAl_2O_4$, Al_2O_3, MgO and $Y_3Al_5O_{12}$ with Ca-Al-silicates containing Mg and Fe in oxidizing, reducing and sulphur-containing atmospheres. Electrochemical interaction and decomposition of oxides such as ZrO_2 in molten salts and silicates. Effects of grain boundary chemistry and structure, crystallographic structure and electrical characteristics on dissolution and electrochemical reactions. Mass transport and diffusion near reaction interfaces from elemental distributions and grain boundary character using high-resolution, quantitative EDX, electron microprobes and STEM, coupled with optical microscopy, TEM, SEM and AES and related surface analyses.

261. SPUTTER DEPOSITED AMORPHOUS SEMICONDUCTORS

P. M. Martin, W. T. Pawlewicz
Phone: (509)-375-2076
$100,000 01-1

Study of the effects of composition and microstructure on the electrical, optical and mechanical properties in sputtered thin film amorphous semiconductors. Development of models of reaction kinetics and film-plasma interactions occurring during the reactive sputtering process. Exploration of relationships between local bonding and configurations, stoichiometry and microstructure. The properties of SiN:H and Si-N-O being investigated. Measurements of intrinsic stress, bonding, phase composition and stoichiometry. Electrical property determinations of temperature dependent resistivity, Hall effect, C-V and I-V characteristics. Optical properties under investigation are refractive index, infrared vibrational absorptions and the fundamental interband absorption edge. Measurement techniques: optical and infrared spectroscopy, Raman spectroscopy, electrical transport measurements, C-V and I-V analysis, XPS, X-ray diffraction and X-ray fluorescence.

LABORATORIES

PACIFIC NORTHWEST LABORATORY (continued)

262. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

R. H. Jones, M. T. Thomas, D. R. Baer, M. J. Danielson
Phone: (509)-376-4276
$360,000 01-2

Investigation of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium-nickel and nickel-based alloys in gaseous and aqueous environments. Relationships between grain boundary chemistry, hydrogen embrittlement and intergranular stress corrosion cracking of Fe, Ni and FeCrNi are investigated with surface analytical tools, electrochemical polarization, straining electrode tests, subcritical crack growth tests and crack tip and fracture surface analysis. Modeling of the electrochemical conditions at the tip of a growing crack and evaluation of the electrochemical behavior of sulfur and phosphorus in the grain boundaries of nickel. Effect of plastic strain and various gaseous environments (O_2, H_2O and H_2O + Cl) on the quantity and distribution of surface adsorbates on Fe, Ni and FeCrNi is being studied by Auger Electron Spectroscopy using an in-situ straining stage.

263. OXIDATION AND CORROSION RESISTANT FINE-GRAINED MATERIALS

J. T. Prater, D. R. Baer
Phone: (509)-375-6905
$65,000 01-3

Investigations of the mechanisms controlling the high-temperature corrosion of sputter-deposited fine-grained materials. Oxidation and sulfidation studies on stainless steel in $CO-CO_2$ and $CO-CO_2-H_2S$ gaseous environments at 800 to 1000C. AEM, micro-focus x-ray diffraction and mechanical tests are being used to determine the effect alloy grain size, alloying additions, and gaseous environment have on scale microstructure, scale adherence and scale cracking behavior. AES, XPS, and nuclear microprobe measurements are employed to determine the diffusion and chemical state of elements at the alloy surface during the corrosion process.

PACIFIC NORTHWEST LABORTORY (continued)

264. LEACHING OF GLASS AND CERAMICS

G. L. McVay, L. R. Pederson, D. S. Goldman
Phone: (509)-375-3762
$250,000 01-3

Mechanistic studies of the interactions of silicate glasses and crystalline ceramics with water, by systematic variation of bulk structure, surface properties, and solution chemistry. Structural studies consider the influence of bridging/nonbridging oxygen ratios, extent of polymerization, and redox effects on leachability. Surface electrical properties in solution, sorption phenomena, and the nature of an altered surface layer are included in studies of the effects of surface properties on leaching. Solution chemistry parameters of interest include pH, Eh, ionic strength, saturation with respect to key glass components, and the use of isotopically-labelled water.

265. RADIATION EFFECTS IN METALS AND CERAMICS

E. P. Simonen, J. L. Brimhall, G. J. Exarhos, E. R. Bradley,
L. A. Charlot, C. H. Henager Jr., H. E. Kissinger, R. Wang,
W. J. Weber
Phone: (FTS) 444-3124
$650,000 01-4

Evaluation of radiation damage mechanisms in metals and non-metals; irradiation of metals using heavy-ion and neutron bombardment; analyses using analytical electron microscopy, positron annihilation, rate theory microstructural modeling; in-situ irradiation creep testing; effects of irradiation and substructure on creep, recovery, recrystallization, defect microstructures and hardening; pulsed irradiation effects on microstructures; effects of primary damage on amorphous and crystalline phase stability and corrosion resistance; studies of ferritics, nickel, molybdenum, amorphous metals, and ordered intermetallic compounds. Dose and dose rate dependence of damage ingrowth in non-metallic solids resulting from internal alpha decay events, external ion bombardment, and gamma irradiation. Characterization of localized defect states in glasses and crystals by vibrational Raman spectroscopy and optical absorption techniques. Kinetic studies of damage ingrowth and annealing phenomena using x-ray diffraction, electron microscopy, and bulk swelling determinations. Model development for the damage state in insulators with an emphasis on radiation induced structural changes in glassy silicates and phosphates.

LABORATORIES

PACIFIC NORTHWEST LABORATORY (continued)

266. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR

R. W. Knoll
Phone: (509)-375-6902
$90,000 01-5

Synthesis of metallic alloys, ceramic, and dielectric materials by sputter deposition and reactive sputtering. Characterization of microstructure, structure and phase stability, using x-ray diffraction, TEM, SEM, AES, thermal analysis, as well as electrical and optical measurements. Emphasis on unique nonequilibrium or metastable phases and composites. Definition of the deposition process and relations between process parameters and material characteristics. Material systems include rare earth/transition metal alloys, refractory metal alloys, binary and ternary oxides.

267. THIN FILM OPTICAL MATERIALS

W. T. Pawlewicz, J. W. Griffin, P. M. Martin
Phone: (509)-375-2074
$270,000 02-2

Measurement, modeling and improved understanding of the optical and materials properties of oxides, nitrides and elemental semiconductors in single and multilayer thin-film form. Materials synthesis by reactive sputtering. Optical properties studied: absorption, scattering, optical homogeneity and isotropy, spectral dependence of complex refractive index, and fundamental interband and lattice vibrational absorption edges. Related materials properties: structure, microstructure, bonding in amorphous materials, stoichiometry, composition, purity, surface topography and mechanical stress. Optical measurement techniques: total integrated scattering, angular scattering distribution, reflectance and transmission spectrophotometry, photoacoustic spectroscopy, laser interferometry and ellipsometry. Materials characterization emphasis on X-ray diffraction, Raman spectroscopy and scanning transmission microscopy. Performance environments: high-power lasers, solar radiation, temperature cycling and humidity exposure.

LABORATORIES

SANDIA NATIONAL LABORATORIES
P. O. Box 5800
Albuquerque, New Mexico 87185

F. L. Vook - Phone: (FTS) 844-9304 or (505)-844-9304

275. ION IMPLANTATION AND DEFECTS IN MATERIALS

P. S. Peercy, S. T. Picraux, S. M. Myers, K. L. Brower,
B. L. Doyle, H. J. Stein, D. M. Follstaedt, J. A. Knapp,
W. R. Wampler, L. E. Pope, F. G. Yost, R. B. Diegle, N. R. Sorensen
Phone: (FTS) 844-4309 or (505)-844-4309
$850,000 01-3

Ion implantation in conjunction with laser and electron-beam annealing to form metastable and equilibrium states within the near-surface regions of metals, semiconductors, and insulators. Microscopic characterization of modified layers by ion-beam depth-profiling, ion channeling, TEM, EPR, AES, ESCA, optical absorption and X-ray scattering. Studies of kinetics of transient laser/electron-beam annealing by time-resolved reflectance and conductance and by calorimetry. Diffusion rates, phase diagrams, and solute-trapping mechanisms in equilibrium intermetallic systems. New metastable crystalline and amorphous alloys produced both by ion implantation and by transient annealing; stability bounds, microstructures, and mechanical and corrosion properties are measured. Ion implantation used to separate structural and chemical effects on corrosion. Methods based on ion implantation and ion beam analysis used to characterize the behavior of hydrogen in metals, including diffusivity, solubility, surface-barrier effects, and trapping by defects, solutes, precipitates and gas bubbles. Fundamental properties of defects and impurities in semiconductors using EPR and optical absorption following controlled introduction by ion implantation. Laser and electron-beam annealing of silicon for the removal of implantation-doping damage, the production of single-crystal silicon on insulators, and to elucidate fundamental aspects of rapid solidification. Refractory amorphous alloys for diffusion barriers or metallization of semiconductors for elevated temperature applications.

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE(continued)

276. STRESS CORROSION IN CERAMICS AND SOL GEL TRANSITION IN SIMPLE SILICATES

T. A. Michalske, M. L. Knotek, G. A. Fisk, B. C. Bunker,
K. D. Keefer, D. W. Schaefer, C. J. Brinker
Phone: (FTS) 844-4069 or (505)-844-4069
$500,000 01-2

Multidisciplinary studies to relate molecular structure of ceramics to physical properties. Develop models for environment/strained solid interactions used to interpret fatigue effects; Electron Stimulated Desorption (ESD) and Photon Stimulated Desorption (PSD) of in situ fracture surfaces to determine chemical compounds resulting from stress corrosion fracture; tunable IR laser used to excite specific molecular adsorbate vibrations during crack growth; molecular orbital (MO) calculations used to predict reactivity of mechanically strained crack tip bonds; model systems to study strain-enhanced chemistry; FTIR studies of adsorbate reactions used to relate strain enhanced chemistry and stress corrosion fracture. Characterize sol-to-gel and gel-to-glass transitions in the silica system using SAXS, HPLC, NMR, and light scattering to determine structures of the pre-gel phase, random colloidal aggregates, and the gel-to-glass conversion; model structure of porous materials using concepts of fractal geometry to predict structure solid material from solution chemistry, and model sintering and absorption characteristics of random porous materials.

277. STRAINED-LAYER SUPERLATTICE MATERIALS SCIENCE

R. M. Biefeld, L. R. Dawson, I. J. Fritz, P. L. Gourley,
D. R. Myers, G. C. Osbourn
Phone: (FTS) 844-6653 or (505)-844-6653
$350,000 01-5

Studies of strained-layer superlattices (SLS's), a new class of semiconductor materials with unique and tailorable electronic and structural properties are expected to have a broad range of device applications. Research emphasizes: electronic energy levels and the effects of Brillouin zone folding on optical transition strengths in SLSs; transport properties and quantum oscillations in SLS structures tailored for large mobilities; conditions for growth and doping of new SLS structures; stability of SLS's subjected to high temperature aging, ion implantation damage and annealing, thermal cycling, and hydrostatic pressure.

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE (continued)

278. SURFACE PHYSICS RESEARCH AND STIMULATED DESORPTION

M. L. Knotek, J. E. Houston, D. Jennison, G. Kellogg, R. R. Rye,
R. Stulen, J. Kelber, A. Burns
Phone: (FTS) 844-2272 or (505)-844-2272
$690,000 02-2

Broad program with wide technological and scientific impact involving experimental and theoretical studies aimed at understanding the interaction of solid surfaces with their environment; unique local surface Properties obtained by exploiting Auger Electron Spectroscopy, Photon and Electron Stimulated Desorption Spectroscopies, the Pulsed Laser Atom-Probe technique and Low Energy Electron Loss Spectroscopy. Studies from those on the chemical nature and local electronic properties of intermediate species adsorbed on catalytic surfaces to work determining the molecular properties controlling initiation sensitivity in aromatic explosives; from studies of the chemistry of oxide surfaces and its relationship to catalytic support interactions and stress corrosion cracking in glasses and ceramics to work dealing with the effect of microscopic surface defects on the interaction of adsorbates with metal surfaces. Theoretical work complements several of these experimental efforts by elucidating the physics of the processes involved to provide a better understanding of the relationship between the results and fundamental material properties.

279. ORGANIC CONDUCTORS AND SUPERCONDUCTORS

L. J. Azevedo, D. S. Ginley, J. F. Kwak, P. J. Nigrey,
J. E. Schirber
Phone: (FTS) 846-2529 or (505)-846-2529
$300,000 02-2

The fundamental physical properties of the charge transfer organic superconductors and the polymeric organic conductors. Directed toward understanding the detailed band structure, doping, and carrier transport in these materials, especially as they pertain to understanding metal-insulator transitions, superconductivity, and the role of disorder in determining transport properties. Unique and specialized instrumental capabilities including high frequency magnetic resonance, conductivity, photoconductivity, thermal conductivity, heat capacity, magnetotransport, de Haas van Alphen, thermopower and tunneling. Experiments at temperatures as low as 0.05 K, magnetic fields up to 120 kOe and hydrostatic pressure to 10 kbar in various combinations. An active in-house synthesis program in collaboration with J. Williams at Argonne National Laboratory supports the measurement programs and develops new materials. The in-house synthesis of novel charge transfer organic superconductors and the chemical and electrochemical growth of very high purity polymeric organic conductors.

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE (continued)

280. CHEMICAL VAPOR DEPOSITION AND SURFACE PHOTOKINETIC RESEARCH

A. W. Johnson, W. G. Breiland, P. Ho, M. E. Coltrin,
J. R. Creighton, P. J. Hargis, M. E. Riley
Phone: (FTS) 844-8782 or (502)-844-8782
$410,000 03-3

Studies of important vapor-phase reactions and nucleation processes during CVD deposition under conditions used to fabricate photovoltaic cells, corrosion-resistant coatings, and semiconductor devices. Measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Test of our predictive model, which includes chemical kinetics and fluid dynamics. Study and development of laser CVD, laser photochemical deposition, laser-based physical deposition, and laser-based fabrication of small-dimension structures. Application of our laser-based measurement capabilities to the study of vapor phase reactions of these laser processing techniques and application of surface measurement techniques to study the product materials. Fundamental study of the interactions of photons and molecules near and on surfaces. Auger, Sims and laser-based measurements of surfaces during deposition and etching. Development of model for combined laser, admolecule, and surface dynamics.

LABORATORIES

SANDIA NATIONAL LABORATORIES
Livermore, California 94550

D. Hartley - Phone (FTS) 532-2747 or 412-422-2747

290. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION-RELATED MATERIALS

R. E. Palmer, J. C. Hamilton, A. S. Nagelberg
Phone: (FTS) 532-3126 or (415)-422-3126
$390,000 01-1

Investigations in real time of gas-solid reactions, emphasizing hot corrosion and microstructural effects in attack of metals and ceramics. Studies of molten alkali sulfate-vanadate attack of yttria-stabilized zirconia. Role of surface microstructure on reaction processes determined in situ with a hot stage on a Raman microprobe. Temporally resolved corrosion studies with mixed gas-phase oxidants in environmental cells. Program relies heavily on Raman spectroscopy to characterize reaction conditions difficult to analyze by post-exposure techniques.

291. GASES IN METALS

M. I. Baskes, G. J. Thomas, M. S. Daw
Phone: (FTS) 532-3226 or (415)-422-3226
$249,000 01-2

Investigations of the behavior of hydrogen and helium in metals involving joint theoretical and experimental research. Experimental techniques include electron microscopy, positron annihilation, mechanical property measurements, and small angle neutron scattering, applied to tritiated metals and also metals implanted with helium below the damage threshold. Theoretical effort on spontaneous lattice damage by helium and on helium-dislocation interactions. A new theoretical method (Embedded Atom Method) developed to calculate the cohesive energy of metals and alloys with chemically active impurities which is being used to investigate the atomistic processes of fracture and the effects of hydrogen and trapping of hydrogen by impurities and alloying additions.

SANDIA NATIONAL LABORATORIES - LIVERMORE (continued)

292. MECHANISMS OF HYDROGEN EMBRITTLEMENT - EFFECTS OF GASEOUS VERSUS ELECTROCHEMICAL CHARGING

S. L. Robinson, N. R. Moody, J. C. Farmer
Phone: (FTS) 532-2209 or (415)-532-2209
$120,000 01-2

Investigation of electrochemical charging with hydrogen to simulate gaseous hydrogen environments by comparing electrochemically and gas phase charged FCC alloys. Electrochemical charging experiments using poisoned, unpoisoned and tritium labelled electrolytes and gas phase charging experiments using hydrogen and tritium atmospheres. Electrochemical techniques of cathodic polarization, cyclic voltammetry and impedance to characterize surface response to charging conditions and solutions. Ion beam profiling determines hydrogen depth profiles, effective hydrogen diffusivities, and effective hydrogen fugacities. Autoradiography of tritium charged samples characterizes hydrogen interactions with microstructural features. Scanning and transmission electron microscopy techniques determine the type of microstructural damage induced by electrochemical and gas phase charging techniques and the conditions which induce damage.

293. THIN SURFACE LAYER REACTIONS

R. E. Palmer, R. J. Anderson, J. C. Hamilton
Phone: (FTS) 532-3126 or (415)-422-3126
$230,000 02-2

In situ studies of the early stages of oxide and other compound formation on metal surfaces. Characterization of bond structure of few-monolayer surface films, time evolution of this bond structure to crystalline structure, and atomic mobility during film thickening. Studies of the role of temperature and oxygen partial pressure in rearrangement rates and final film structures. Primary measurement technique is spontaneous Raman spectroscopy, complemented by Auger spectroscopy and LEED. Development of greater capability of Raman for detecting very thin, possibly monolayer, or weakly scattering oxide films by means including electronic resonant enhancement and state-of-the-art instrumentation. Raman spectroscopy of films tagged with oxygen isotopes to determine reaction mechanisms.

LABORATORIES

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

C. S. Smith - Phone (FTS) 327-7180 or 303-231-7180

Materials Research Branch - 01 -
G. E. Gross - Phone (FTS) 327-1228 or 303-231-1228

295. POLYMER/THIN-FILM PHOTO AND CATALYTIC DEGRADATION RESEARCH

A. W. Czanderna, P. Schissel, J. D. Webb, J. R. Pitts
Phone: (303)-231-1240
$290,000 01-1

Photo and catalytic degradation mechanisms of polymeric materials exposed to simulated and enhanced solar environments in the presence and absence of supported thin films; stability of polymer/thin film interfaces; studies of polymethylmethacrylate, polycarbonate, and polypropylene in contact with copper and silver oxides, chlorides, and sulfides or copper, silver, and gold; UV radiation, environmental oxidizing gases, and atmospheric pressures; interfacial catalytic effects and photodegradative effects; FT-IR reflection absorption spectroscopy, UV-vis spectroscopy, λ, GPC, XPS, ISS, SIMS, AES, SEM, excimer/dye laser, solar simulator.

Solid State Research Branch - 02 -
S. Deb - Phone (FTS) 327-1105 or 303-231-1105

296. SEMICONDUCTOR THEORY

A. Zunger
Phone: (303)-231-1172
$130,000 02-3

Theoretical study of electronic and structural properties of new semiconductors for optoelectronic applications to clarify electronic properties, predict new materials, characterize structurally-driven optical and electronic phenomena. Systems: ternary chalcopyrites ABC_2 (A=Cu, B=Al, Ga, In, C=S,Tr); ternary pnictides ABC_2 (A=Zn, B=Si, Ge, Sm, C=P, As); and ternary alloys of binary semiconductors $A_xB_{1-x}C$. Theoretical techniques: all-electron Mixed Basis Potential Variation (MBPV) band structure method, and non-local pseudopotential method. Study of the properties of deep defects in semiconductors to establish chemical trends in 3d impurity levels, predict hitherto unobserved levels, clarify role of deep impurities on material characteristics as affecting their use in optoelectronic devices. Systems: Si, III-V and II-VI semiconductors. Theoretical techniques: Quasi Band Crystal Field (QBCF) Green's function method, and Modified ("effective Δ") multiplet theory.

LABORATORIES

STANFORD SYNCHROTRON RADIATION LABORATORY
Stanford University
P. O. Box 4349, Bin 69
Stanford, California 94305

A. I. Bienenstock - Phone (FTS) 461-9300 or (415) 854-3300

298. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES (see also page D-13)

A. I. Bienenstock, G. S. Brown, and H. Winick
Phone: (FTS) 461-9300 or (415) 854-3300
$700,000 02-2

Research and development on insertion devices and other equipment and facilities to improve research capabilities of synchrotron radiation sources.

SECTION B

Contract and Grant Research

(Primarily Universities)

The information in this Section was prepared by the DOE project monitors of the Division of Materials Sciences. There is considerable turnover in the Contract and Grant Research program and some of the projects will not be continued beyond the current contract period. (The Division is in the process of changing its mode of funding basic research from contracts to grants. No distinction is made between these modes in this Section.)

ARIZONA STATE UNIVERSITY
Tempe, AZ 85281

301. TRANSPORT IN SOLID ELECTROLYTES CONTAINING A DISPERSED SECOND PHASE

J. B. Wagner
Center for Solid State Science
Phone: (602)-965-6959, 4544

$84,917 (18 Months) 01-3

Characterization of contribution of number and mobility of ionic charge carriers and of space charge layers to conductivity increase mechanisms in a AgI or CuCl matrix containing a second phase such as silica, MgO, flyash, etc. Role of aliovalent doping of the matrix phase. Behavioral effects due to moisture and to added dielectrics such as alcohols or hydrocarbons. SEM, variable frequency ac conductivity, and dc polarization analysis.

302. IMAGING OF SURFACES AND DEFECTS OF CRYSTALS

J. M. Cowley
Dept. of Physics
Phone: (602)-965-6459

$105,879 02-2

Techniques of microdiffraction, imaging of surfaces using reflected diffracted electrons and electron energy loss spectroscopy applied to study of near-amorphous thin films of oxides and other corrosion products on metal surfaces and investigations of surface reactions of various ceramic oxides. Allied development and exploration of new and improved electron-optical techniques for study of surface structures and reactions and the influence of crystal defects.

UNIVERSITY OF ARIZONA
Tucson, Arizona 85721

303. ARTIFICIALLY LAYERED SUPERCONDUCTORS

C. M. Falco
Dept. of Physics
Phone: (602)-626-1866

$75,141 02-2

Investigation of the structure of artificial metallic multilayer systems, their electronic and superconducting properties including their weak link characteristics; produce superlattices with higher perfection than theretofore; understand what are the important preparation parameters. Fabricate layered materials with a three-gun magnetron sputtering system and use x-ray diffraction, resistance, Rutherford backscattering, TEM, electron tunneling to characterize the samples. Emphasis on the superconducting properties of the superlattice systems to develop weak links and microbridges with increased range of operating conditions.

BATTELLE COLUMBUS LABORATORIES
505 King Avenue
Columbus, OH 43201

304. MULTIAXIAL STRESS RESPONSE OF CERAMICS

A. R. Rosenfield
Phone: (614)-424-4353
D. K. Shetty
Phone: (614)-424-4353
S. G. Sampath
Phone: (614)-424-4353
W. H. Duckworth

$160,000 01-5

Response of ceramic materials to multiaxial stress states. Consideration of: (a) surface conditions, (b) test geometry, and (c) environment. Control of each of the above variables so individual effects can be studied. Specimen preparation to insure that the flaw population is isotopic and materials directionality is eliminated. Relationship of stress-state effects to stress-intensity factor, effects of tensile and shear stresses parallel to an artificial crack and effect of stress ratios on strength in ceramic specimens containing natural flaws to evaluate statistical (Weibull) descriptions of strength. Material characterization, fractrography, three-dimensional linear elastic finite element analysis of test-specimen geometries and stress-intensity factors. High-temperature biaxial tension tests of ceramic specimens containing controlled artificial flaws. Materials of interest: AL_2O_3, SiC, Si_3N_4, and glass-ceramics, and partially stabilized ZrO_2.

BOEING AEROSPACE COMPANY
P. O. Box 3999
Seattle, WA 98124

305. X-RAY SPECTROSCOPIC INVESTIGATION OF METAMICTIZATION & ANNEALING IN CRYSTALLINE PHOSPHATES, SILICATES AND COMPLEX TI-NB-TA OXIDES

R. B. Greegor
Phone: (206)-655-0514
F. W. Lytle
Phone: (206)-655-5574

$80,030 01-1

Detailed examination of the near neighbor site geometries of metal atoms in metamic minerals (e.g., A (U,TH) and B (Ti,Nb,Ta) site cations) as determined by extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) spectroscopy performed at the SSRL. Study of radiation damage annealing and leaching mechanisms of metamict minerals. Determination of the structure of the metamict state. Assessment of long-term stability of crystalline titanate, phosphate, and silicate radioactive wasteforms (e.g., SYNROC, Sandia Titanate) which would be subject to the same processes of radiation damage and geochemical alteration in applications as a primary host for radioactive wastes.

BRANDEIS UNIVERSITY
415 South Street
Waltham, MA 02254

306. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

R. B. Meyer
Dept. of Physics
Phone: (617)-647-2231

$43,955 02-2

Experimental study of two-dimensional structures formed by interfacial and thin-layer colloids, especially with regard to two-dimensional melting. These colloidal systems exhibit truly two-dimensional behavior, free of periodic substrate interactions. The particle scale (0.1 to 10μm) permits both exploration of reciprocal space by coherent light scattering and direct real space observations by optical microscopy.

BROWN UNIVERSITY
Providence, RI 02912

307. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS

R. J. Asaro
Div. of Engineering
Phone: (401)-863-1456
J. Gurland
Div. of Engineering
Phone: (401)-863-2628
A. Needleman
Div. of Engineering
Phone: (401)-863-2863
C. F. Shih

$237,000 01-2

Theoretical and experimental studies of fracture in metals, principally steels; combined theoretical and experimental studies of crack tip deformation and micro-fracture processes at crack tips; finite element modelling of crack tip behavior including studies of yield surface vertices on crack tip fields; correlations of microstructure and fracture toughness of dual phase and quenched and tempered martensitic steels; time dependent crack tip deformation and finite element modelling of creep deformation at crack tips; applications to engineering fracture mechanics; hydrogen assisted fractures in steels.

BROWN UNIVERSITY (continued)

308. CONCURRENT USE OF STRESS PULSES AND ULTRASONIC WAVES TO STUDY EFFECTS OF RAPID STRAIN ON THE INTERNAL STRUCTURE OF SOLIDS

C. Elbaum
Div. of Applied Mathematics
Phone: (401)-863-2186
A. Hikata
Div. of Applied Mathematics
Phone: (401)-863-2187

$93,500 01-2

Measurement of deformation of metals at intermediate strain rates $(10^{-1}-10^{3} \text{ sec}^{-1})$, using the Hopkinson bar method for generating stress wave and ultrasonic methods to monitor the materials response; relationships between stress, mobile dislocation density, average velocity, and strain rate under single as well as multiple slip conditions; dislocation interaction with point effects; metals studied - Al, Fe, Nb, Ti, Zn.

309. CHARACTERISTICS OF THE ROLE OF CYCLIC COMPRESSIVE LOADS IN THE GROWTH OF FATIGUE CRACKS IN STEELS

S. Suresh
Div. of Engineering
Phone: (401)-863-2626

$94,950 01-2

Experimental study of the influence of compression cycles on the growth of cracks in steels under constant and variable amplitude fatigue loading conditions; modelling of the micromechanisms of cyclic crack advance under continuous and periodic compression loading. Analyses of the role of crack closure as a function of microstructure, load ratio, and environment under far-field cyclic compression.

310. NOVEL DYNAMIC INVESTIGATIONS OF EXCITONS AND THEIR STRUCTURE IN SEMICONDUCTORS

A. V. Nurmikko
Div. of Engineering
Phone: (401)-863-2869

$80,444 02-2

Characteristics and energetics of excitons in selected semiconductors studied from a dynamical point of view. Subnanosecond laser sources and transient spectroscopy used to obtain new information about energy relaxation and localization and the effect of screening of an interacting excitonic gas. Materials include Cu_2O and (Zn, Mn)Te mixed crystals.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA 91125

311. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

W. L. Johnson
Div. of Engineering and Applied Science
Phone: (818)-356-4433
$270,000 01-1

Synthesis, structure, and properties of amorphous alloys, the principal aim of which is to understand the thermodynamics and kinetics of phase transformations in, and the structure of noncrystalline materials. Characterization of the electronic structure of metallic glasses and its relation to atomic structure, and investigating the formation of glassy materials not prepared by rapid quenching. Atomic structure studies include use of EXAFS, XANES, SAXS, SANS, X-ray Raman scattering, Mossbauer spectroscopy, and NMR. Electronic structure is probed by measuring specific heats, transport properties and superconductivity.

312. MELTING IN ADSORBED FILMS

D. Goodstein
Div. of Physics, Mathematics, and Astronomy
Phone: (213)-356-4315
$93,000 02-2

Experimental study of the relation between dimensionality and phase transitions, especially melting, in multilayer adsorbed films. Comprehensive thermodynamic measurements together with pulsed nuclear magnetic resonance is used to study the interaction of melting with wetting, roughening and other surface related phenomena. A prototypical study: multilayer methane adsorbed on graphite foam.

UNIVERSITY OF CALIFORNIA/DAVIS
Davis, CA 95616

313. RADIATION DAMAGE AND STABILITY OF NUCLEAR WASTE STORAGE MATERIALS

D. G. Howitt
Dept. of Mechanical Engineering
Phone: (916)-752-1164, 0580
$97,000 01-1

Evaluation of fundamental processes of radiation damage in silicate based glasses and the leaching behavior of multicomponent glasses and ceramics. Concerns include the chemical role of helium in the radiation damage process, the size of damage volumes involved in the crystalline to amorphous transformation, and the radiation damage processes that contribute to the radiolytic decomposition of cements.

UNIVERSITY OF CALIFORNIA/DAVIS (continued)

314. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY

A. K. Mukherjee
Dept. of Mechanical Engineering
Phone: (916)-752-1776

$59,746 01-2

Experimental study of superplastic deformation of metals, microduplex steels and Al-base alloys; correlation between mechanical behavior (e.g., stress, strain rate, temperature) and microstructure (e.g., grain size, dislocation structure and precipitate morphology); identification of superplastic and creep mechanisms; analysis of cavitation behavior and its implication to superplastic forming.

315. AN INVESTIGATION OF THE ROLE OF SINTERING IN GAS-SOLID INTERACTIONS

Z. A. Munir
Dept. of Mechanical Engineering
Phone: (916)-752-0559

$66,000 01-3

Investigation of the role of sintering in the kinetics of gas-solid interactions in powder compacts, including both oxidation-reduction and dissociation reactions. Study of state of division of oxide ceramic resulting from the decompostion of hydroxides and carbonates as a function of gas pressure, temperature, and impurities. Evaluation of changes of oxide particle shape and size as a function of sintering parameters. Morphological changes such as surface area, pore size, and overall porosity are measured and related to changes in the reversibility and rates of reactions. The role of sintering is elucidated by thermogravimetric, microscopy, and surface area measurement techniques.

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, CA 92717

316. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

J. C. Hemminger
Dept. of Chemistry
Phone: (714)-833-6020
S. Ushioda
Dept. of Physics
Phone: (714)-833-6619

$140,000 02-2

Combine Raman spectroscopy and modern surface science technology to study binding and chemistry of adsorbates on well characterized surfaces. Study mechanism of "giant" enhanced Raman scattering. Correlate enhancement with surface roughness on stepped and kinked surface of Ag. Also correlate enhancement with electronic energy levels of metal-adsorbate system as determined by electron energy loss spectroscopy. Apply Raman spectroscopy to study of corrosion by H_2S and O_2.

317. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

D. L. Mills
Dept. of Physics
Phone: (714)-833-5148

$103,000 02-2

Theory of electron energy loss spectroscopy (EELS) and other inelastic scattering at surfaces. Vibrational properties of isolated adatoms and ordered overlayers on metal surfaces, with emphasis on quantitative comparisons with experiment. Role of image potential in large-angle EELS and in LEED studies. Large-angle inelastic scattering from substrate phonons. EELS spectral densities at large wave vector. Surface relaxation, anharmonicity, and surface lattice dynamics. This program strongly coupled to that of S. Y. Tong, University of Wisconsin-Milwaukee.

UNIVERSITY OF CALIFORNIA/SAN DIEGO
La Jolla, CA 92037

318. INVESTIGATION OF THE INTERACTION BETWEEN SUPERCONDUCTIVITY AND MAGNETISM AND OSCILLATORY CHEMICAL REACTIONS OVER METAL SURFACES

M. B. Maple
Dept. of Physics
Phone: (714)-452-3969

$292,000 02-2

An experimental program to investigate the coexistence of superconductivity and magnetism. A-15's, ternary molybdenum chalcogenides, and other high T_c superconductors of primary interest. Properties of rare earth compounds such as $ErRh_4B_4$ and $ErMo_6Se_8$ studied in order to understand re-entrant and coexistence phenomena. Collaborative efforts study valance instabilities in Ce compounds and the superconductivity of graphite intercalated with potassium. Studies of the oscillatory oxidation of CO on Pt using LEED and Auger techniques and of metallic thin film oxidation using electrical resistance.

319. ION MIXING AND SURFACE MODIFICATION IN METAL SEMICONDUCTOR SYSTEMS

S. S. Lau
Dept. of Electrical Engineering and Computer Sciences
Phone: (619)-452-3097
D. M. Scott
Dept. of Electrical Engineering and Computer Sciences
Phone: (619)-452-3428

$157,195 02-4

Investigation of the physical mechanisms responsible for ion-mixing effects in metal-semiconductor systems. Generalize and predict ion-induced reactions, correlations between ion-induced reactions and those induced by conventional thermal annealing are established and the physical mechanisms and conditions necessary for the formation of a specific reaction product are determined. Different metal-Si systems are investigated; sample configurations include single metal layer on Si bilayers, multi-layers, and alloy thin film structures. Primary experimental tools are ion implantation, thermal annealing, Rutherford backscattering, Auger electron spectroscopy, X-ray diffraction, and transmission electron spectroscopy. A collaborative program between the University of California, San Diego, and Cornell University and involves interaction with Oak Ridge National Laboratory.

UNIVERSITY OF CALIFORNIA/SAN DIEGO (continued)

320. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

J. C. Wheatley
Dept. of Physics
Phone: (505)-667-7499

$146,214 02-5

Fundamental investigations in thermal physics: (a) quantitative scientific properties of intrinsically irreversible acoustic engines, of other "natural engines" based on the same principles, and of engines using liquid working substance; (b) thermal convection in dilute solutions of ^{3}He in superfluid ^{4}He emphasizing quantitatively the steady convection, highly periodic oscillatory convection, and both the deterministic and stochastic chaos which can develop; (c) the production of spin polarized atomic hydrogen isotopes from a low temperature source together with measurement of physical properties using magnetosound; and (d) study of magnetism in superfluid ^{3}He-A, especially ferromagnetism in zero magnetic field and magnetic anisotropy in small applied fields.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

Santa Barbara, CA 93106

321. CONDENSED MATTER RESEARCH USING THE UCSB FREE ELECTRON LASER

V. Jaccarino
Dept. of Physics
Phone: (805)-961-2121
L. Elias
Dept. of Physics
Phone: (805)-961-4387

$130,000 02-2

Initiate the first use of a Free Electron Laser(FEL) for materials research in the United States. This unique device is a source of high-intensity coherent but pulsed electromagnetic radiation tunable over the wavelength range of 50 to 2000 micrometers. Research on the nonlinear phenomena of phonons, and other excitations after development of techniques and facilities.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

322. RESEARCH ON THE THEORY OF PATTERN FORMATION IN SYSTEMS FAR FROM EQUILIBRIUM

J. S. Langer
Dept. of Physics
Phone: (805)-961-4111

$109,629 02-3

Theory of pattern formation in systems far from equilibrium. Specific studies of boundary-layer model of dendritic solidification, theory of pattern selection in directional solidification of alloys, and statistical theory of the kinetics of phase separation. The pattern-forming processes studied of primary importance in the design of metallurgical materials, but applications in other areas also considered.

323. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino
Physics Dept.
Phone: (805)-961-2871
J. R. Schrieffer
Physics Dept.
Phone: (805)-961-3061
R. L. Sugar
Physics Dept.
Phone: (805)-961-4078

$160,000 (21 Months) 02-3

Development of stochastic numerical techniques for simulating many-body problems where the particles obey Fermi statistics. One-dimensional systems investigated considering various electron-phonon interactions to further the fundamental understanding of conducting polymers. One-dimensional chains of quantum mechanical spins studied with application to spin glasses and pseudo random spin systems such as $CeNiF_3$. Correlation effects and frequency dependent transport considered to test the validity of theoretical approximations such as the Pade and Pade-conformal map techniques. Consideration of many-fermion systems in two and three spatial dimensions.

CARNEGIE INSTITUTION OF WASHINGTON
Washington, DC 20008

324. STUDY OF THE PROPERTIES OF HYDROGEN AT STATIC PRESSURES OF ONE MEGABAR

P. M. Bell
Geophysical Laboratory
Phone: (202)-966-0334
H. K. Mao
Geophysical Laboratory
Phone: (202)-966-0334
$60,000 02-2

Investigations of the hydrogen isotopes, helium, neon, argon, carbon dioxide, methane and other simple gases under very high prssure. Hydrogen studies at static pressure above 2 Mbar. Laser Raman scattering studies of the molecular bonding phenomena and the elastic constants as a function of pressure in deuterium. Further improvement to the Diamond Anvil Cell technique. The Raman and Infrared spectra, Brillouin and X-ray scattering measurements on solid hydrogen and solid argon.

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

325. THE EFFECT OF STRESS ON PRECIPITATE MORPHOLOGY

W. Johnson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-8785
D. Laughlin
Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-2706
$92,211 01-1

Theoretical and experimental study of second phase morphology changes, owing to misfit strains and applied stress. System parameters include, misfit strains, volume fraction, nature of applied stress, differences in elastic constants. Theoretical approach uses bifurcation theory. Alloys that may be studied: Ni-Al, Al-Li, Cu-Co. Experimental techniques include electron microscopy, X-ray diffraction.

CARNEGIE MELLON UNIVERSITY (continued)

326. THE ROLE OF PASSIVE SURFACE FILMS ON CORROSION FATIGUE CRACK

I. M. Bernstein
Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-2700
A. W. Thompson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-2711
G. W. Warren
Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-3517

$104,599 01-2

Effects of microstructure and nature of passive surface films on corrosion fatigue crack initiation; heat treatment developed to change the microstructure and thus the degree of slip planarity in A286, a superalloy stainless steel; potentiostatic and potentiodynamic techniques used to demonstrate that the alloy forms a stable passive film in various aqueous solutions, highly resistant to pitting; repassivation kinetics determined in scratch tests; electrochemical results are being analyzed using existing and developed current buildup and decay models; experiments underway to measure fatigue-induced crack initiation rates under controlled electrochemical conditions, comparing these to similar tests run in air and in inert environments.

CASE WESTERN RESERVE UNIVERSITY
Cleveland, OH 44106

327. MICROSTRUCTURE-MECHANICAL PROPERTY RELATIONSHIPS IN TRANSFORMATION-TOUGHENED CERAMICS

A. H. Heuer
Dept. of Metallurgy and Materials Science
Phone: (216)-368-3868

$142,000 01-2

Ostwald ripening in ZrO_2 toughened Al_2O_3. Plastic deformation in two phase "single crystal" Ca partially-stabilized ZrO_2, and in 100 percent tetragonal ZRO_2 polycrystals. Stress-induced transformation in Y-TZP and ZTA. The focus of these studies will be the nature and extent of the transformation zone associated with propagating cracks and the critical factors involved in processing strong and tough polycrystalline tetragonal ZrO_2. Correlation of TEM analysis with mechanical properties.

CASE WESTERN RESERVE UNIVERSITY (continued)

328. COUPLED DIFFUSION PHENOMENA

A. R. Cooper
Dept. of Metallurgy and Materials Science
Phone: (416)-368-4224

$66,756 (24 Months) 01-3

Study of rate processes, e.g., precipitation, dissolution, and phase separation in multicomponent systems at high temperatures. Study of transport processes and thermodynamics in multicomponent molten silicate systems, and kinetics of these processes in such systems. Relation of the inter-diffusion coefficient matrix to the individual ionic species mobilities or self-diffusion coefficients. Work focused on systems K_2O-SrO-SiO_2 and CaO-Al_2O_3-SiO_2. Ultimate goal is a sufficiently well-documented understanding of such transport processes that will be useful for prediction of behavior in the many high temperature processes that involve molten silicates.

UNIVERSITY OF CHICAGO
5801 S. Ellis Avenue
Chicago, IL 60639

329. RESEARCH IN THE THEORY OF CONDENSED MATTER AND ELEMENTARY PARTICLES

L. P. Kadanoff
The James Franck Institute
Phone: (312)-962-7189
Y. Nambu
The James Franck Institute
Phone: (312)-962-7286
D. Friedan
Dept. of Physics
Phone: (312)-962-7119
S. Shenker
Dept. of Physics
Phone: (312)-962-7187

$161,314 02-3

Theoretical research on problems relevant to both elementary particle physics, through quantum field theory, and condensed matter physics, via the statistical mechanics of phase transitions. Topics of current interest: non-linear dynamical systems and the transition to chaos, dendritic growth, parallel processing computers as statistical mechanical systems, chiral symmetry breaking in lattice gauge theories, quantized string theory (free and interacting), and problems of chial fermions in lattice theories.

CLARK COLLEGE
Atlanta, GA 30314

330. INVESTIGATIONS OF CHARGE TRANSPORT IN THE THERMOELECTRET STATE OF SOME GLASSES AND CERAMICS

O. P. Puri
Dept. of Natural Sciences and Mathematics
Phone: (404)-681-3080 X200
$93,910 01-3

Investigation of the mechanism of formation and decay of electrets in nonpolar inorganic polycrystalline and amorphous dielectrics. Experimental characterization of electret formation with sample temperature, polarization field, and cooling rate, and of electrect formation with sample temperature, polarization field, and cooling rate, and of electret decay in the open and closed circuit condition. Extension of Swann-Gubkin theory by considering the nonpolar part of electret polarization through the displacement of ions to account for the production through the displacement of ions to account for the production of nonpolar electrets. Materials of interest include $CaTiO_3$, $SrTiO_3$, BaO_4, TiO_2, $BiTiO_3$, $(SrBi)TiO_3$, chalcogenide glasses and elemental Se. X-ray diffraction. Thermally stimulated discharge current analysis.

COLORADO SCHOOL OF MINES
Golden, CO 80401

331. MICROSTRUCTURE AND PROPERTIES OF FERROUS ALLOY WELDMENTS

D. L. Olson
Dept. of Metallurgical Engineering
Phone: (303)-273-3787
D. K. Matlock
Dept. of Metallurgical Engineering
Phone: (303)-273-3775
$155,718 01-5

Role of Al, Cr, C and N additions on the phase stability and transformation in single pass and multiple pass Fe-Mn-Ni weld metal. Gleeble testing of Fe-Mn-Ni-Al alloys. Determination of martensite start temperature for high alloy ferrous (cryogenic) weld metal. New analytical expressions (based on fundamental concepts) for predicting weld metal microstructure and properties. Impression creep testing and modeling of heterogeneous materials (weldments). Creep behavior in heterogeneous material. High temperature mechanical degradation of ferritic-austentic dissimilar metal weldments.

UNIVERSITY OF COLORADO
Boulder, CO 80309

332. LIGHT SCATTERING STUDIES OF LOWER DIMENSIONAL COLLOIDAL PARTICLE AND CRITICAL FLUID SYSTEMS

W. O'Sullivan
Dept. of Physics
Phone: (303)-492-7457
R. Mockler
Dept. of Physics
Phone: (303)-492-8511

\$188,000 (18 Months) 02-2

Quasi-elastic light scattering (QELS), microscopy, and various other optical techniques used to study charged colloidal particle suspensions (CCPS) in thin films, in monolayers, and on bilipid membranes. Examination of melting/crystallization dynamics in CCPS films, supercooling of CCPS liquid films, recovery from electric field induced non-equilibrium states in CCPS films, monolayers and membranes, melting/crystallization, diffusion, order-disorder phenomena for CCPS in monolayers and on membranes, and development of a model of the interaction between colloidal particles in monolayers and on membranes. Also the application of innovative QELS techniques to study the transition to two dimensional behavior of the critical dynamics of thin fluid films.

COLUMBIA UNIVERSITY
New York, NY 10027

333. DEFECT INTERACTIONS AT HIGH CONCENTRATION IN SOLID OXIDE ELECTROLYTES

A. S. Nowick
Henry Krumb School of Mines
Phone: (212)-280-2921

\$87,295 01-3

Defects and their interactions in oxygen-ion solid electrolytes, with special emphasis on ceria-based materials doped with divalent and trivalent cations. Techniques used include ionic conductivity, dielectric relaxation, anelastic relaxation, neutron diffraction and scanning transmission electron microscopy. Defect interactions in trivalent-doped (M^{3+}) ceria and effect of M^{3+} ion radius. Role of silicon phases in producing electrical blocking at grain boundaries. Steps that control the electrode reaction, particularly at Pt electrodes. Protonic conduction studies in $SrCeO_3$, and $KTaO_3$.

UNIVERSITY OF CONNECTICUT
Storrs, CT 06268

334. THE FATIGUE BEHAVIOR OF FERRITIC STEELS AT ELEVATED TEMPERATURES

A. J. McEvily
Dept. of Metallurgy and Institute of Materials Science
Phone: (203)-486-2941
$60,540 01-2

Creep-fatigue-environmental behavior of ferritic steels (9-and 12Cr) related to strength, microstructure, oxidation resistance, fracture mechanics parameters. Influence of hold times and frequency in air and in vacuum. Determination of dominant failure mode, i.e., creep or fatigue. Modeling of the fatigue crack growth process based on range of crack opening displacement and crack closure mechanisms. Effect of temperature and mean stress on closure. Short crack growth. Fatigue crack growth in weldments. Creep crack growth.

335. ELECTRODE STUDIES IN MOLTEN SALTS

O. F. Devereux
Dept. of Metallurgy and Institute of Materials Science
Phone: (203)-486-4620
$47,611 01-3

Deterioration of refractory oxide films on Ni and Fe in sulfide-bearing molten salts. Field and anion effects; 'electrochemical' dissolution of oxides. Film thinning, pore formation, and structure change evaluation by impedance techniques. Formation of anodic chromium sulfides in molten sulfide salts. Current-potential characteristics of anodic sulfide films.

336. INVESTIGATION OF ROLE OF SUBSURFACE ZONES IN WEAR OF MATERIALS

R. Solecki
Dept. of Mechanical Engineering
Phone: (203)-486-2366
$89,500 (24 Months) 01-5

Experimental characterization of the formation, composition and morphology of both subsurface zones and wear debris for materials pairs making solid contact both in sliding and repetitive impact modes; experimental investigation of the roles of nominal contact stress, relative sliding velocity and effective contact stiffness of subsurface zone formation, composition and morphology; analytical prediction of the equilibrium configuration of subsurface morphology for a work hardening elastoplastic material subject to given load cycling and temperature distributions; model development which allows prediction of composition and morphology of subsurface zones for selected materials subjected to both sliding and impulsive contact; and postulation and experimental investigation of in situ development of wear resistance.

UNIVERSITY OF CONNECTICUT (continued)

337. ENERGY TRANSFER & NONLINEAR OPTICAL PROPERTIES AT NEAR ULTRAVIOLET WAVELENGTHS: RARE EARTH 4F-5D TRANSITIONS IN CRYSTALS & GLASSES

D. S. Hamilton
Dept. of Physics and Institute of Materials Science
Phone: (203)-486-3856
$61,172 02-2

The optical properties of rare-earth-doped crystals and glasses which involve the near-ultraviolet 4f-5d transitions of the dopant ions investigated using transient and steady state optical spectroscopy. Optical properties include multiphoton absorption, energy transfer, population dynamics, photo-ionization, phase conjugate wave generation, and excited-state absorption and gain.

CORNELL UNIVERSITY
Ithaca, NY 14853

338. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL PROPERTIES OF POLYCRYSTALLINE SILICON FILMS

D. G. Ast
Dept. of Materials Science and Engineering
Phone: (607)-256-4140
$92,900 (20 Months) 01-1

Characterization of the structure (high resolution TEM, electron diffraction) and electrical properties (EBIC, LIBIC, I-V, DLTS) of diffusion bonded ("welded") and as grown grain boundaries; relationship between boundary structure (esp. symmetry) and electrical activity, CSL theory, broken bond models; interactions between twins and dislocations during growth and cooling of ribbon crystals; influence of carbon (present at solubility limit in all graphite crucible grown Si) on Si self interstitial mobility, electrical activity; carbon precipitation based gettering cycles of chemical impurities.

339. THE MIGRATION OF GRAIN BOUNDARIES IN CERAMICS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

C. B. Carter
Dept. of Materials Science and Engineering
Phone: (607)-256-4797
$99,000 01-1

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic and covalent solids. Concerns include (a) misorientation between grains and boundary plane orientation, (b) geometry of interfacial dislocations and steps, (c) interfacial chemistry including local segregation and nonstoichiometry, and (d) interfacial pinning by pores or crystalline or amorphous pockets or films of a second phase. Materials of investigation include Al_2O_3, MgO, NiO, Mg-Al spinel, Si, Ge, Si_3N_4 and SiC. Studies on both powder compacts and bicrystals involve visible light microscopy, electron microprobe analysis, and strong- and weak-beam, lattice fringe, X-ray energy dispersive, and electron energy loss TEM analysis.

CORNELL UNIVERSITY (continued)

340. DIFFRACTION AND MICROSCOPY STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES IN FE, FE-BASE ALLOYS, AND CERAMIC MATERIALS

S. L. Sass
Dept. of Materials Science and Engineering
Phone: (607)-256-5239

$174,000	01-1

Investigation of grain boundary structure of BCC metals and ceramics using transmission electron microscopy and x-ray diffraction techniques; study of the influence of segregation on the structure of grain boundaries in Fe-base alloys; study of facet structure of tilt grain boundaries in NiO; model diffraction observations from grain boundary region to determine changes in plane spacing normal to interface in NiO and MgO; relation of structural observations on grain boundaries to mechanical properties.

341. AN INVESTIGATION OF MECHANICAL BEHAVIOUR OF POLYCRYSTALLINE SOLIDS

C-Y. Li
Dept. of Materials Science and Engineering
Phone: (607)-256-4349

$190,000	01-2

State-variable description of nonelastic deformation and related phenomena in polycrystalline solids. Extensive use is made of load relaxation experiments of combinations of load relaxation and stress-dip experiments spanning strain rates from 10^{-8} to $10^{2}.s^{-1}$ and low to high ($T > T_m/2$) homologous temperatures. Efforts to relate microstructurally or physically based theories to various state variables are embodied in the program as well as parallel efforts to incorporate these constitutive relations into complex stress, deformation, and structural design analyses.

342. EXPERIMENTS AND MICROMECHANICAL MODELS FOR CREEP-RUPTURE IN POLYMER-MATRIX COMPOSITES

S. L. Phoenix
Sibley School of Mechanical and Aerospace Engineering
Phone: (607)-256-3462

$105,000	01-2

Theoretical modelling and experimentation for the strength and creep-rupture lifetime of unidirectional composites; statistical/micromechanical models wherein fibers fail due to randomly distributed flaws; local stress redistribution among contiguous fibers halts fracture propagation; time dependence through viscoelasticity in the matrix leading to local creep and stochastic decay in fiber strength from thermally induced flaw growth; calculation of short-term strength and long-term lifetime probability distributions using direct, recursive and asymptotic techniques; creep-rupture experiments on "microcomposites" of about 20 parallel fibers impregnated with matrices varying widely in creep properties; fibers are Kevlar 49 (aramid), S-glass and carbon; matrices are epoxy, polyester, polyethylene and nylon 6; special equipment constructed for fabricating and testing such composites.

CORNELL UNIVERSITY (continued)

343. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE

R. Raj
Dept. of Materials Science and Engineering
Phone: (607)-256-4040
$99,000 01-2

Elucidation of the mechanisms of densification and flaw generation during high-temperature processing of powder compacts with inhomogeneous microstructures. Influence of agglomerates, non-uniform packing and second phase constituents on the densification process. Fundamental investigation of diffusion bonding of two ceramic surfaces with the aid of a liquid phase. Free sintering, hot-pressing, and sintering under superimposed hydrostatic pressure experiments on Al_2O_3 (model material for dry processing) and Si_3N_4 (with a liquid phase additive for wet processing). Diffusion bonding of like and unlike ceramics with the aid of a liquid phase.

CORNING GLASS WORKS
Sullivan Park
Corning, NY 14830

344. LUMINESCENT GLASS-CERAMICS: OPTICAL SPECTROSCOPIC INVESTIGATIONS

G. H. Beall
Research and Development Div.
Phone: (607)-974-3430
$180,800 02-2

Compositional studies of doped glass-ceramics with potentially useful luminescent behavior. Preparation and characterization of transparent host compounds based on various solid solution crystals and doped with transition metal and rare earth luminescing ions. Properties of interest include nucleating agents, crystallinity, particle size, optical perfection, thermal expansion, and refractive index. Spectroscopic properties, radiative transfer and glass-ceramic structure are evaluated from measurements of absorption, emission and excitation spectra, fluorescence yield, excited-state lifetimes, light scattering, and electron paramagnetic resonance.

DARTMOUTH COLLEGE
Hanover, NH 03755

345. THE STRUCTURE AND MECHANICAL PROPERTIES OF STOICHIOMETRIC Ni_3Al AND OF Ni_3Al ALLOYED WITH BORON

E. M. Schulson
Thayer School of Engineering
Phone: (603)-646-2888

$106,109 01-2

Structure and mechanical properties of stoichiometric Ni_3Al and of Ni_3Al microalloyed with 750ppm boron consolidated from rapidly solidified powders via two and three-stage hot and warm extrusion. Correlation of discontinuous yielding, yield strength, work hardening, ductility and fracture mode in tension (at 77 to 1023 K) with grain size, superlattice dislocations and superlattice faults. Microstructural stability; dynamic recrystallization. Use of conventional and analytical TEM for microstructural examination, XRD for texture determination, SEM-SACP's for fractography and AES for segregation to grain boundaries.

UNIVERSITY OF DELAWARE
Newark, DE 19716

346. DURABILITY OF SHORT FIBER COMPOSITE MATERIALS

T. W. Chou
Dept. of Mechanical and Aerospace Engineering
Phone: (302)-451-2904

$59,756 01-2

Experimental and theoretical investigaton of the durability of short glass and carbon fiber reinforced thermoplastics; strength and fracture behavior of fiber bundle, resin matrix and composites subjected to static and cyclic loadings as well as aggressive environmental attack; measurements of residual strength, failure time and failure characteristics of aligned and partially aligned short fiber composites; characterization of stress-corrosion cracking, fatigue, and corrosion fatigue; determination of fiber-matrix interfacial profile from fracture surface analyses; analytical modeling of the stress-corrosion behavior of fiber bundles and resin matrices, and development of a statistical strength theory for fiber composites; major parameters in analysis include fiber flaw induced stress concentration and concentration of corrosive agents; correlation of experiments with modeling.

UNIVERSITY OF DELAWARE (continued)

347. NEUTRON STUDIES OF LIQUID AND SOLID HELIUM

H. R. Glyde
Dept. of Physics
Phone: (302)-738-2661

$55,000 02-3

A theoretical program to calculate properties of liquid and solid helium for direct comparison with neutron scattering measurements in terms of existing and new models and to propose new experiments. Specific examples include $S(Q,\omega)$ in liquid ^{3}He, the momentum distribution in liquid ^{3}He and solid ^{4}He, and to test the impulse approximation.

UNIVERSITY OF DENVER
Denver, CO 80208

348. CATION DOPANT EFFECT ON THE LATTICE THERMAL EXPANSION OF CORDIERITE

P. K. Predecki
Dept. of Chemistry
Phone: (303)-871-2141

$79,359 01-3

Lattice thermal expansion measurements will be carried out on cordierite doped with alkali and akali earth dopants using high-temperature Guinier diffractometry. Selected samples will be investigated further using neutron powder diffraction at the Argonne IPNS. Results will be correlated to reveal the mechanism of expansion in this structure.

349. THE DETECTION OF HYDROGEN ASSISTED CRACK GROWTH

S. H. Carpenter
Dept. of Physics
Phone: (303)-871-2176

$72,700 01-5

Experimental investigation of new techniques to study the initiation and growth of cracks in hydrogen environment; techniques include continuous measurement of elastic modulus and acoustic emission; materials investigated include pure iron and a number of stainless steels; measurements are carried out at zero load as well as under applied stress; additional measurements of the internal friction provide insight and information on hydrogen-dislocation interactions; acoustic emission tests on small pressure vessels to determine if acoustic emission monitoring can be used on real structure exposed to hydrogen environments.

EMORY UNIVERSITY
Atlanta, GA 30322

350. FAR INFRARED STUDIES OF SUPERCONDUCTING A-15 STRUCTURES, NBN AND NB

S. Perkowitz
Physics Dept.
Phone: (404)-329-6584

$43,901 (24 Months) 02-2

Optical techniques in the far infrared region will be used to explore the basic superconducting behavior of the high temperature superconductors V_3Si, Nb_3Ge, Nb and granular NbN. Such spectroscopy will yield accurate gap values, information about the temperature dependence of superconducting properties, values of the electron-phonon spectral function and insight in to grain-to-grain coupling in inhomogeneous geometries. These results will be used to calculate basic superconducting parameters such as the coupling constant and the transition temperature, T_c, with the aim of explicating the underlying physics of superconductivity.

UNIVERSITY OF FLORIDA
Gainesville, FL 32611

351. MODERATE AND LOW TEMPERATURE OXIDATION OF CLEAN NICKEL, CHROMIUM, AND NI-CR ALLOYS

P. Holloway
Dept. of Materials Science and Engineering
Phone: (904)-392-1461
C. Batich
Dept. of Materials Science and Engineering
Phone: (904)-392-1461

$115,000 01-3

Investigation of low and moderate temperature ($100\ K \leq T \leq 800\ K$) oxidation of atomically clean single and polycrystalline Ni, Cr and Ni-Cr alloys. Surface segregation studies by Auger electron, X-ray photoelectron and ion scattering spectroscopies. Oxidation kinetics and adsorbed states characterization in ultra-high vacuum (UHV) with X-ray photoelectron spectroscopy, scanning Auger electron spectroscopy, low energy and reflection high-energy electron diffraction (LEED and RHEED), work function changes and temperature desorption spectroscopy. Oxide structure analysis with LEED, RHEED and transmission electron microscopy. The oxygen pressure will be varied from 10^{-10} Torr to 1 atmosphere, with higher pressure exposures being accomplished in a reaction chamber external to the UHV chamber. Specific aspects of the oxidation to be studied include oxide nucleation, lateral oxide growth to form a coalesced layer, thickening of the coalesced oxide layer, dissolution of the oxygen into the bulk and the effect of controlled oxide microstructure upon high temperature oxidation. This study will directly investigate the phenomena occurring in the transition from an atomically clean surface to a thick oxide at elevated temperatures.

UNIVERSITY OF FLORIDA (continued)

352. FIELD-ION MICROSCOPY AND SPECTROSCOPY OF HYDROGEN IN METALS

J. J. Hren
Dept. of Materials Science and Engineering
Phone: (904)-392-6985
$76,290 01-3

Investigation of hydrogen trapping sites and diffusion in BCC and FCC metals (Nb and Ni, respectively) using TEM and field ion microscopy; pulse desorption to determine trap site energetics; influence of substitutional solutes on above. Implantation of D and He into Ni and Fe emitters at energies up to 20 keV. Characterization of emitters by transmission electron microscopy before and after implantations. Coupling of ion source to imaging atom probe for *in situ* implantation at ∿40-50 K followed by IAP analyses.

353. SYNTHESIS OF MODEL POLYMERS AND RELATED STRUCTURES IN SUPPORT OF VINYL MONOMER GRAFTING STUDIES

T. E. Hogen-Esch
Dept. of Chemistry
Phone: (904)-392-2011
G. B. Butler
Dept. of Chemistry
Phone: (904)-392-2012
$94,000 03-1

The objectives of the proposed research program are to study graft copolymerization of vinyl monomers to polysaccharides, to determine grafting efficiencies, and to determine the structure and properties of the copolymers. In support of these objectives, a variety of model polymers will be synthesized (a) which contain the specific reactive functional groups of the polysaccharide repeating unit, (b) which possess controlled branching sites in order to simulate highly branched polysaccharide grafted copolymers, and (c) which contain macrocyclic units to aid in establishing viscosity-structure relationships.

FRANKLIN INSTITUTE
20th and Parkway
Philadelphia, PA 19103

354. PHYSICS OF HIGHLY ANISOTROPIC MATERIALS

S-T. Chui
Physics Dept.
Phone: (302)-738-8115
$25,005 02-3

Theoretical research on instabilities and elementary excitations associated with correlations in highly anisotropic (mainly quasi-one-dimensional) materials. Principal subject areas: spin and charge density wave relationships, correlations in half filled bands, solitons and Hubbard model excitations, and superconductivity in one-dimensional

GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, GA 30332

355. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDY OF THE GEOMETRY OF SURFACE COMPLEXES

U. Landman
School of Physics
Phone: (404)-894-3368
$159,000 02-3

Theoretical studies of surface phenomena toward fundamental understanding of processes which govern the properties of material surfaces, especially: surface reactivity, surface crystallography, electronic and vibrational structure, dynamical processes, phase transformations and phase changes and the properties of interfaces. Emphasis on surface defects, heterogeneities and reaction mechanisms, surface melting and solidification.

HARVARD UNIVERSITY
Pierce Hall
Cambridge, MA 02138

356. DRIFT MOBILITIES BY TIME-OF-FLIGHT METHODS AND TIME-DEPENDENT PHOTOTRANSPORT IN THE NANOSECOND REGIME IN AMORPHOUS SEMICONDUCTORS

W. Paul
Div. of Applied Sciences
Phone: (617)-495-2853
$120,000 02-2

Time-of-flight measurements in the nanosecond to millisecond regime, and other time-dependent studies of amorphous hydrogenated silicon, doped and undoped, which have been carefully characterized as to their structure, band structure and steady-state electrical and optical properties. A coherent, self-consistent model of transport and recombination processes sought.

357. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

I. F. Silvera
Dept. of Physics
Phone: (617)-495-2872
$260,000 (18 Months) 02-2

Investigation of the properties of the quantum gases of spin-polarized atomic hydrogen and deuterium. Attempt to reach high enough densities and low enough temperature that these unusual gases undergo Einstein-Bose Condensation. If this new form of matter obtained, the expected superfluidity of this weakly interacting gas to be sought and, if found, characterized.

UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE
Chicago, IL 60680

358. OXIDATION OF TRANSITION METALS IN CHLORINE CONTAMINATED ENVIRONMENTS

M. McNallan
Dept. of Civil Engineering, Mechanics and Metallurgy
Phone: (312)-996-2436

$32,400 01-3

Experimental investigation of the oxidation of transition metals (Fe, Ni, Co) in mixed gas environments containing oxygen and chlorine. Thermogravimetric measurement of corrosion kinetics. Analysis of corrosion product morphologies and chemistries using optical and electron microscopy. Interpretation of corrosion mechanisms in mixed gas environments containing volatile corrosion products and characterization of corrosion kinetics under these conditions. Behavior described in terms of chlorination, paralinear oxidation, or catastrophic oxidation. Identification of thermodynamic conditions producing latter behavior in each metal.

INDIANA UNIVERSITY
Bloomington, IN 47402

359. HIGH-RESOLUTION ELECTRON ENERGY LOSS STUDIES OF SURFACE VIBRATIONS

L. L. Kesmodel
Dept. of Physics
Phone: (812)-335-0776

$62,725 02-2

Measurements of surface vibrational properties of clean surfaces and of metal-adsorbate systems principally by High-resolution[3-7 meV] Electron Energy Loss Spectroscopy(EELS). Detailed phonon dispersion information is to be obtained on a variety of metal surfaces e.g., palladium, aluminum, copper and gold, and adsorbate elements, such as oxygen. The goal is to better understand the interaction between metal atoms at surfaces and the modifications which accompany adsorption phenomena.

UNIVERSITY OF KENTUCKY
Lexington, KY 40506

360. ANISOTROPIC ELASTICITY OF COALS

P. P. Gillis
Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-257-8884(8882)
A. B. Szwilski
Dept. of Mining Engineering
Phone: (606)-257-2953(8026)

$70,535 01-2

Determination of the anisotropic elastic constants of various coals are correlated with structural properties of various coals in search of valid connections between elastic moduli and other more readily determined materials properties.

UNIVERSITY OF KENTUCKY (continued)

361. STUDIES OF THE MICROSCOPIC PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE INTERCALATION COMPOUNDS

P. C. Eklund
Dept. of Physics and Astronomy
Phone: (606)-257-6725
$94,731 02-2

Experimental research on graphite intercalation compounds, especially with antimony halide and alkali metal intercalates. Techniques include optical reflectance (infrared to VUV), Raman scattering, Mössbauer spectroscopy, X-ray diffraction, neutron scattering, and magnetoresistance.

362. STRUCTURAL CHARACTERIZATION OF DISPERSED METAL CATALYSTS

P. J. Reucroft
Dept. of Metallurgical Engineering
Phone: (606)-257-8723
R. J. De Angelis
Dept. of Metallurgical Engineering
Phone: (606)-257-3238
$82,292 03-3

Structural and morphological studies on small metal crystallites dispersed in porous support phases; influence of interactions between metal and support; metals include nickel, gold, and cobalt; support phases include silica, magnesium silicate, and nylon. Techniques used: analytical electron microscopy, X-ray diffraction, ion scattering spectroscopy, energy dispersive X-ray analysis, and microdiffraction.

LEHIGH UNIVERSITY
Bethlehem, PA 18015

363. ANALYTICAL ELECTRON MICROSCOPY STUDIES OF PRECIPITATION IN CERAMIC SYSTEMS

M. R. Notis, D. B. Williams, and M. P. Harmer
Materials Research Center
Phone: (215)-861-4225
$128,000 01-1

Study of precipitation phenomena by means of analytical and high resolution electron microscopy, laser Raman spectroscopy and X-ray diffraction. Phase transformations resulting in transformation toughening in ZrO_2 containing ceramics. Precipitate dissolution kinetics and transient second phase phenomena in the Y_2O_3-La_2O_3 system. Precipitate coarsening kinetics in NiO and CoO, precipitation processes in mullite and glass ceramic materials.

LEHIGH UNIVERSITY (continued)

364. INVESTIGATIONS OF CREEP CAVITATION IN TYPE 304 STAINLESS STEEL

T. Delph
Dept. of Mechanical Engineering & Mechanics
Phone: (215)-861-4119
$74,145 01-2

Experimental studies of creep cavitation in austenitic stainless steel under uniaxial and multiaxial stress states using automatic image analysis, creep cavitation around notches; statistical analysis of cavitation data; stereological considerations.

365. CORROSION FATIGUE OF SMALL CRACKS: MECHANICS AND CHEMISTRY

R. P. Wei
Dept. of Mechanical Engineering and Mechanics
Phone: (215)-861-3587
$129,430 01-2

Experimental and theoretical study of corrosion fatigue of NiCrMoV and 304 stainless steels in aqueous solutions; kinetics of growth of small fatigue cracks as a function of frequency, solution chemistry, temperature and crack length; electrochemical reaction kinetics as a function of temperature in the same environment; relating fatigue crack growth response to the electrochemical reaction kinetics; modelling of electrochemical conditions near the crack tip and of the electrochemical and micromechanics aspects of small-crack growth.

LOUISIANA STATE UNIVERSITY
Baton Rouge, LA 70803

366. STUDIES OF SUB-MICRON DEVICES WITH EMPHASIS ON MOS SYSTEMS

R. F. O'Connell
Dept. of Physics and Astronomy
Phone: (504)-388-6835
$91,982 (14 Months) 02-3

Theoretical study of electrons in quasi-two-dimensional systems, as relevant to the physics of sub-micron devices. Magneto-optical phenomena in metal-oxide-semiconductor (MOS) systems. Wigner distribution function (WDF) techniques in sub-micron device physics. Strong magnetic and electric field effects in two-dimensional systems.

UNIVERSITY OF MARYLAND
College Park, MD 20742

367. GASES ON METAL SURFACES: ADSORPTION AND PHASE TRANSITIONS

T. L. Einstein
Dept. of Physics
Phone: (301)-454-3419
R. E. Glover III
Dept. of Physics
Phone: (301)-454-3417
R. L. Park
Dept. of Physics
Phone: (301)-454-4127

$194,525 02-2

Joint theoretical/experimental investigation of surface interactions and imperfections which have an important influence on surface reactivity. Studies of oxygen adsorption and reaction at low temperatures on polycrystalline films and single crystal surfaces. Measurements of adatom-adatom interactions with high resolution LEED/Auger to examine the degree of long- and short-range order of chemisorbed layers. Monte Carlo simulations and transfer-matrix-scaling calculations of phase diagrams to obtain interaction parameters. Experimental determination of critical exponents associated with two-dimensional phase transitions and comparison with phase transition theory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, MA 02139

368. GRAIN BOUNDARIES

R. W. Balluffi
Dept. of Materials Science and Engineering
Phone: (617)-253-3349
P. D. Bristowe
Dept. of Materials Science and Engineering
Phone: (617)-253-3326

$328,400 01-1

Investigations of the structure and properties of grain boundaries consisting essentially of a combined computer simulation and experimental attack on the problem of determining the atomic structure and corresponding properties of high-angle grain boundaries in metals and ceramic oxides. Materials studied include MgO, Au, Cu-Al and alloys of Au and Ag. Experimental techniques employed include X-ray diffraction experiments at the NSLS, high-resolution and conventional electron microscopy and computer simulation.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

369. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS

W. D. Kingery
Dept. of Materials Science and Engineering
Phone: (617)-253-3319
R. L. Coble
Dept. of Materials Science and Engineering
Phone: (617)-253-3318
$685,000 01-1

Electrical and optical behavior of Al_2O_3 and MgO, including vacuum ultraviolet spectroscopy characterization of band gaps. Float zone laser crystal growth and zone refining in Al_2O_3 and grain boundary migration in high purity powder and bicrystals of Al_2O_3. Kinetic studies include oxygen diffusion measurements in MgO by gas exchange and SIMS, reaction processes and microstructure development in low-temperature sub-solidus systems, rapid quenching effects in a eutectic Ca-Mg-silicate liquid phase and the Fe-Cu two phase system, suppression of insulator charging in SEM and SIMS measurements, grain boundary diffusion in $SrTiO_3$, and Bi and O grain boundary diffusion in ZnO. Defect structures, defect interaction, grain boundary and surface studies include point defects in SiC, B and C distribution in doped SiC, grain boundary microchemistry and slow crack growth in SiC, influence of microstructure and grain boundary segregation on electrical properties of polycrystalline ZnO, grain boundary segregation in polycrystalline Al_2O_3, segregation at special grain boundaries in MgO, influence at grain boundary composition on grain boundary diffusion, structure of a migrating low angle tilt grain boundary in $SrTiO_3$, and role of grain boundary segregation on high temperature deformation in SiC and Al_2O_3. Sintering studies include atom transport, processing and sintering of SiC, grain boundary mobility in alkali halides, test of the applicability of Herring's scaling law, the effect of MgO on sintering of Al_2O_3, and orientation effects on the grain boundary migration of high purity Al_2O_3.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

370. MECHANISMS OF TRANSFORMATION TOUGHENING

G. B. Olson
Dept. of Materials Science and Engineering
Phone: (617)-253-6901
I. W. Chen
Dept. of Materials Science and Engineering
Phone: (617)-253-7100
A. S. Argon
Dept. of Mechanical Engineering
Phone: (617)-253-2217

$166,145 01-2

Development of constitutive flow relations for transformation plasticity based on nucleation-controlled martensitic transformation kinetics in both homogeneous and dispersed-phase composite materials; critical experiments on specially-designed model materials in metals (high-strength austenitic and martensitic steels), ceramics (ZrO_2 and alkali halide dispersed-phase composites), and metallic glasses; influence of stress-state, strain-rate, and temperature; determination of nucleation site potency distributions and influence on flow behavior; TEM study of nucleation in ZrO_2 small-particle bicrystals; application of constitutive relations in crack-tip plasticity calculations as a basis for toughening.

371. RAPIDLY SOLIDIFIED CERAMICS

G. Kalonji
Dept. of Materials Science and Engineering
Phone: (617)-253-6863
R. O'Handley
Dept. of Materials Science and Engineering
Phone: (617)-253-6913

$129,980 01-3

Rapid solidification studies of the systems Al_2O_3-ZrO_2, Al_2O_3-MgO, Y_2O_3-ZrO_2, selected ternary compositions from the previous binary systems, Ba ferrite, and Ni-Zn ferrite. Sample preparation by means of a 1500 watt CO_2 laser to melt feed rods of the desired composition, melt spinning, 1000 watt CO_2 laser to perform surface melting and regrowth experiments at controlled solid-liquid interface velocities, and ultrasonic atomization. Sample characterization by means of STEM, XRD, EXAFS, IR and Raman spectroscopy, vibrating sample magnetometry and B-H hysteresis loops and magnetic permeability for soft ferrites.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

372. BASIC MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS

G. J. Yurek
Dept. of Materials Science and Engineering
Phone: (617)-253-3239
$145,000 01-3

Effects of temperature and oxygen partial pressure on the kinetics of growth of Cr_2O_3 scales on pure Cr and Fe-Cr alloys. Defect structure and diffusion mechanisms in Cr_2O_3 scales. Effect of oxide grain growth on the kinetics of growth of oxide scales. Early stages of the oxidation/sulfidation of Cr and Fe-Cr alloys in H_2-H_2O-H_2S gas mixtures. Factors controlling the transition for nonprotective to protective scaling of alloys in sulfur-bearing environments. Oxidation behavior of polycrystalline, rapidly solidified Fe-Cr-Si and Fe-Cr-Ni-Si alloys. Oxidation kinetics determined by thermogravimetry. Characterization of alloys and scales by SEM, TEM/STEM, EPMA, AES/ESCA and XRD.

373. IRRADIATION DAMAGE MICROSTRUCTURES IN NUCLEAR CERAMICS WITH APPLICATION IN FUSION ENERGY TECHNOLOGY AND NUCLEAR WASTE DISPOSAL

L. W. Hobbs
Ceramics and Materials Science Dept.
Phone: (617)-253-6835
$141,103 01-4

Fundamental research to characterize the irradiation stability and radiation damage microstructure of crystalline ceramic solids with application to nuclear energy production and disposal of high-level nuclear waste. The principal mode of investigation is transmission electron microscopy. Materials to be examined include BeO, $MgO.nAl_2O_3$, CaF_2, PuO_2, ZrO_2, SiC, Si_3N_4, Li_2O, $LiAlO_2$, $LiAl_5O_8$, Li_2ZrO_3, $Ca(Zr,Pu)Ti_2O_7$, titanate pyrochlores, SiO_2, GeO_2, $ZrSiO_4$. Neutron, ion and electron irradiation damage will be studied, including the effects of massive recoil nuclei and fission fragments.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

374. INTERFACIAL AND COLLOIDAL ASPECTS OF AQUEOUS SUSPENSIONS CONTAINING OXIDIC POWDERS

A. Bleier
Dept. of Materials Science and Engineering
Phone: (617)-253-6877

$95,000 (27 1/2 Months) 01-5

Application of colloid-chemical models of single and multimetallic oxides to the processing of their powders. Extension of such models to heterogeneous systems containing more than one particle (composition) type, so as to improve understanding of interfacial complexation and related phenomena which influence dispersibility and packing behavior. Objectives include preparation of model, colloidal single and multimetallic oxides using established synthesis routes, characterization of these oxides using crystallographic, chemical, physical, and surface-chemical procedures, and evaluation of the Davis, James and Leckie model of the electrical double layer.

375. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

H. K. Bowen
Dept. of Materials Science and Engineering
Phone: (617)-253-6892

$136,000 01-5

Development of a scientific basis for the processing and packing behavior of the model sub-micron ceramic powders SiO_2, TiO_2, and SiC. Synthesis aspects of the colloid chemistry and mono-sized particle masses. Colloid coagulation. Surface chemistry and powder characterization. Ordering behavior of particulate assemblies. Effects of particle size distribution on slurry stability. Dispersion, packing, and sintering behavior. Generalization controlling the presintered structure of compacts containing 10^{12} particles. Laser diffraction. Photon correlation spectroscopy.

376. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

C. G. Shull
Dept. of Physics
Phone: (617)-253-4812

$316,930 02-1

Fundamental experiments in neutron diffraction and interferometry using the MIT research reactor, such as the analogue of the famous optical Fizeau experiment in which fringe shifts are observed when light is sent through a moving medium; neutrons entering a crystal at an exact Bragg angle propagate through the crystal along the Bragg planes at a drift velocity much less than the group velocity. Ways are sought to exploit this effect. Ways are sought to use neutron interferometry to test nonlinear variants of wave mechanics. Effect of interferometer rotation; nature of coherent wave front in interferometer; single and multiple slit Fresnel diffraction patterns.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

377. MODIFICATION OF THE PROPERTIES OF BENZENE-DERIVED GRAPHITE FIBERS BY INTERCALATION AND IMPLANTATION

M. S. Dresselhaus
Center for Materials Science and Engineering
Phone: (617)-253-6864
G. F. Dresselhaus
Center for Materials Science and Engineering
Phone: (617)-253-6827
$130,000 (24 Months) 02-2

A comprehensive study of the structure and property relationships of benzene-derived fibers, both in their pristine form and as modified by intercalation and implantation. Structural, mechanical and electrical properties of these fibers approach those of graphite single crystals--superior to those of fibers formed by other techniques. Emphasis on characterization by high resolution TEM to identify defects introduced by intercalation and implantation.

378. IMPROVEMENT IN HIGH MAGNETIC FIELD BEHAVIOR OF VANADIUM-GALLIUM SUPERCONDUCTORS BY ENHANCEMENT OF SPIN ORBIT SCATTERING

R. H. Meservey and P. M. Tedrow
Francis Bitter National Magnet Laboratory
Phone: (617)-253-5578
$132,469 02-2

The A15 compound V_3Ga is the best known superconducting material for the fabrication of practical high field magnets. Its usefulness is, however, restricted to about 25T. This is believed to be due to the low spin-orbit scattering because of the low Z elemental components. Two approaches to increasing the spin-orbit scattering will be taken by this program--the inclusion of randomly placed high Z elements with minimum lattice distortion and thin closely spaced high Z material layers. Samples will be prepared by electron beam evaporation and characterized by the superconducting properties, resistivity and spin-polarized tunneling measurements. These measurements will test existing theoretical concepts and are expected to advance the understanding of high field superconductors as well as the role of many-body effects in normal transition metal systems and the development of improved magnetic solenoids.

UNIVERSITY OF MASSACHUSETTS
Amherst, MA 01003

379. ERROSION OF STRUCTURAL CERAMICS

J. E. Ritter Jr.
Dept. of Mechanical Engineering
Phone: (413)-545-0632, (413)-235-2414
K. Jakus
Dept. of Mechanical Engineering
Phone: (413)-545-2424

$38,570 (24 Months) 01-5

Erosion behavior and related strength degradation of Al_2O_3, Si_3N_4, and SiC at temperatures to 1200°C. Assessment of erosion models for predicting erosion behavior and associated strength degradation. Effect of eroding particle velocity, size, angle of impingement, temperature of environment, and subcritical crack growth on erosion rate and related strength degradation for Al_2O_3, SiC and Si_3N_4. Biaxial strength characterizations of as-prepared and eroded samples.

380. SYNTHESIS OF METASTABLE SUPERCONDUCTING COMPOUNDS BY ION IMPLANTATION AND ELECTRON BEAM MELTING AND SPIN QUENCHING

M. T. Clapp
Dept. of Mechanical Engineering
Phone: (413)-545-0868

$35,000 02-2

Ion implantation and spin quench formed metastable A-15 and amorphous superconducting materials. Ion implantation to optimize stoichiometry and to introduce selected impurities. Spin quenching used as a rapid solidification technique for amorphous materials. Furnace and electron beam annealing used to remove radiation damage in implanted samples and to crystallize amorphous preparations. Material forms: Nb_3Al, implanted with B and C; Nb_3Si and Nb_3Ge, implanted with C, N, and O.

MICHIGAN STATE UNIVERSITY
East Lansing, MI 60439

381. STUDIES ON AGE-HARDENING IN SPINODALLY MODULATED ALLOYS-EXPERIMENTAL AND THEORETICAL

K. N. Subramanian
Dept. of Metallurgy, Mechanics & Materials Science
Phone: (513)-353-5197
$60,652 01-2

Structure-property relationship and age-hardening of the spinodal alloy system Cu-10%Ni-6%Sn. Single crystal studies of mechanical properties of both one dimensionally and three dimensionally modulated alloys. Dislocation mobility studies by in-situ HVEM (with deformation stage) experiments. Application and development of elasticity and hardening theories to various multi-phase morphologies associated with the spinodal decomposition reaction. Computer analysis of the energetics of dislocation double-kink formation and for thermally activated dislocation motion. Experiments and theory concerning temperature and strain-rate dependent mechanical behavior.

MICHIGAN TECHNOLOGICAL UNIVERSITY
Houghton, MI 49931

382. ENVIRONMENT-INDUCED EMBRITTLEMENT: EFFECTS OF IMPURITY SEGREGATION AND STATE OF STRESS

L. A. Heldt
Dept. of Metallurgical Engineering
Phone: (906)-487-2630
D. A. Koss
Dept. of Metallurgical Engineering
Phone: (906)-487-2170
$94,000 01-2

Hydrogen embrittlement and stress corrosion cracking with concern for the effects of (a) intergranular misorientation and segregation, (b) local chemistry variation, (c) multiaxial states of stress on such behavior. Experimental methods include (a) bicrystal studies, (b) Auger electron spectroscopy, (c) slow strain-rate testing, and (d) multiaxial deformation and fracture tests.

UNIVERSITY OF MICHIGAN
Ann Arbor, MI 48109

383. EFFECT OF MICROSTRUCTURE ON THE MECHANICAL PROPERTIES OF SILICON NITRIDE CERAMICS

T. Y. Tien
Dept. of Materials & Metallurgical Engineering
Phone: (313)-764-9449, 7489

$92,000 01-1

Study of role and mechanism of nucleating agents on the crystallization of the Si_2N_2O containing grain boundary phases which are formed during the processing of Si_3N_4 (containing Y_2O_3 and Al_2O_3) and SIALON ceramics including SIALON-Cordierite. Microstructure and phase identification in transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

384. A SYSTEMATIC APPROACH TO INTERGRANULAR CRACKING MECHANISMS IN AUSTENITIC ALLOYS THROUGH GRAIN BOUNDARY CHEMISTRY CONTROL

G. S. Was
Dept. of Nuclear Engineering
Phone: (313)-763-4675

$84,000 01-2

Determination of the role of grain boundary chemistry; chromium depletion, carbide precipitation and phosphorous segregation, taken individually and collectively, on intergranular corrosion, stress corrosion cracking and hydrogen embrittlement of P and C doped Ni-Cr-Fe alloys. Grain boundary composition (Cr and P) and carbide distribution monitored by STEM and AES. corrosion testing techniques; potentiodynamic polarization scans, electrochemical potentiokinetic reactivation and constant extension rate testing.

385. SURFACE-PLASMON EXPLORATION OF MULTILAYER PHYSISORBED AND CHEMISORBED FILMS ON METAL SUBSTRATES

M. Bretz
Dept. of Physics
Phone: (313)-764-4494

$75,000 02-2

Measurement of dielectric properties of adsorbed films by laser excitation of surface plasmons. Technique permits study of phase transitions in monolayer to multilayer films following layer-by-layer evolution of films from two to three dimensions, detection of orientational effects of non-spherical adsorbed molecules, and study of a variety of other surface phenomena.

UNIVERSITY OF MINNESOTA
128 Pleasant Street, S.E.
Minneapolis, MN 55104

386. CORROSION RESEARCH CENTER

R. A. Oriani
Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4864
D. A. Shores
Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4183
W. H. Smyrl
Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-2763
$540,000 01-1

Basic research and technology transfer in corrosion. Electron transfer at solid-electrolyte interface and capacitance. In-situ IR spectroscopy at the solid-liquid interface. Study of passivating films by inelastic electron tunneling spectroscopy, rotating ring-disc electrode, electrochemical oscillations, and their destruction by mechanical and chemical effects. Photoelectrochemistry and electrochemical oscillation, and their destruction by mechanical and chemical effects. Photoelectrochemistry and electroluminescence of oxides. Dissolution kinetics of oxide films. Surface microtopography and corrosion of GaAs. Cathodic reduction of hydrogen. Corrosion protection by conducting organic polymers. In situ measurement of stresses in oxide scales by energy dispersive X-ray diffraction, and of their relaxation by acoustic emission. Mechanism of break-down of oxide coatings in relation to parameters.

387. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS

W. W. Gerberich
Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4829
$86,369 01-2

Time- and temperature-dependent effects on fatigue threshold in polycrystalline metals. Investigation of influence of closure as well as internal resistance on crack advance in Fe-Si and Fe-Ni single- and polycrystalline materials. Intrinsic variables: frequency and temperature dependence, dislocation substructure. Extrinsic variables affecting closure: dwell-time and mean stress. Load ratio effects on cyclic cleavage with and without hydrogen. Novel techniques: acoustic emission in conjunction with programmed mechanical loading to understand discontinuous cracking; electron channeling to analyse near-surface deformation.

UNIVERSITY OF MINNESOTA (continued)

388. VERY LOW TEMPERATURE STUDIES OF HYPERFINE EFFECTS IN METALS

W. Weyhmann
School of Physics and Astronomy
Phone: (612)-373-5481

$78,723	02-2

Nuclei, through hyperfine coupling, used as a probe of magnetic interactions in metallic systems; emphasis on the role of conduction electrons. Nuclear singlet ground state intermetallic compounds, very dilute magnetic impurities in non-magnetic metals, and itinerant ferromagnets. Development of the sub-millikelvin refrigeration capabilities of first type and utilization in study of local moment in manganese-based Kondo systems at millikelvin and submillikelvin temperatures. The local magnetization measured with nuclear orientation and the macroscopic magnetization measured with SQUID magnetometry. Search for electron polarization effects in itinerant ferromagnets using nuclear orientation.

UNIVERSITY OF MISSOURI AT KANSAS CITY
1110 E. 48th Street
Kansas City, MO 64110

389. THEORETICAL STUDIES ON THE STRUCTURE OF INSULATING AND METALLIC GLASSES

W-Y. Ching
Dept. of Physics
Phone: (816)-276-1604

$69,345	01-1

Theoretical study of atomic scale, electronic, and dynamic structure of insulating and metallic glasses. Construction of structure models for various noncrystalline solids with periodic boundary conditions. First-principles quantum mechanical calculations of electronic states and vibrational spectra, with emphasis on microscopic information on the localization of electron states and their correlations to the short-range order of the model structure. Approach is to perform exact microscopic OLCAO calculations for the eigenvalues and eigenvectors for model Hamiltonians corresponding to model structures with one to two hundred atoms and periodic boundary conditions.

UNIVERSITY OF MISSOURI
Columbia, MO 65211

390. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES

H. E. Anderson
Dept. of Ceramic Engineering
Phone: (314)-341-4886

	$116,000	01-3

Interrelationship of electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n type transition metal oxides TiO_2, $SrTiO_3$, and $BaTiO_3$, and p type transition metal oxides Cr_2O_3, NiO, $LaCrO_3$, and $YCrO_3$. Experimental aspects include specimens preparation, thermogravimetric measurements, x-ray diffraction, transmission electron microscopy, and ERR magnetic susceptibility, Hall, conductivity, and seebeck measurements.

391. MEASUREMENTS TO VERIFY BRAGG DIFFRACTION AND TOTAL REFLECTION AT A NARROW NUCLEAR RESONANCE

R. M. Brugger
Research Reactor Facility
Phone: (314)-882-4211

	$76,996 (24 Months)	02-1

Measurement of resonance Bragg diffraction of neutrons of several important isotopes that have potential use at pulsed spallation neutron sources. A search for crystals suitable as monochromators and filter detectors. Studies of total reflection at resonance for a few selected isotopes for use as neutron mirrors in the epithermal region.

392. PHOTOCONDUCTIVITY AND EMISSION FROM THE IMPURITY EXCITED STATES IN SILICON

H. R. Chandrasekhar
Dept. of Physics and Astronomy
Phone: (314)-882-6086

	$48,051	02-2

Investigation of excited states in silicon via selective population of these states by tunable laser excitation while simultaneously probing sample materials by means of photoconductivity or emission spectroscopy. Excitation and recombination rates measured and used in identifying the impurity excited states. Effects due to resonant interactions between localized phonons and the impurity states or the electronic continuum also studied. Expect to establish the feasibility of a new type of extrinsic detector of infrared in the 200-100μm range.

UNIVERSITY OF MISSOURI (continued)

393. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MOSSBAUER RADIATION

W. B. Yelon
Dept. of Physics
Phone: (314)-882-4211
G. Schupp
Dept. of Physics
Phone: (314)-882-4211
J. G. Mullen
Dept. of Physics
Phone: (317)-494-3031

$175,000 (19 Months) 02-2

A variety of condensed matter science experiments using the unique source of Tungsten-183 46.5 keV Mossbauer radiation at the University of Missouri. The intensity of the available radiation is about one thousand times more intense than that used in most Mossbauer Spectroscopy, and a special Microscopic Conversion Electron (MICE) detector to be developed and employed. Experiments to separate the elastic and inelastic scattering at Bragg reflections, to determine the quasielastic linewidths observed in critical phenomena and studies of very low energy Landau excitations.

NATIONAL ACADEMY OF SCIENCES
2101 Constitution Avenue
Washington, DC 20418

394. SUPPORT OF A COMMITTEE ON MAJOR FACILITIES FOR MATERIALS SCIENCES

W. Spindel
Commission on Physical Sciences, Mathematics and Resources
Phone: (202)-334-2156

$100,000 02-2

Support for a Committee, chaired by Dr. Frederick Seitz, to establish priorities for major facilities for materials sciences, in response to a request from Dr. George Keyworth, the President's Science Advisor, and Dr. Frank Press, President of the National Academy of Sciences.

UNIVERSITY OF NEVADA
Reno, Nevada 89557

395. INVESTIGATIONS OF TRIPLET EXCITON PROCESSES OCCURRING IN PURE POLYMER FILMS

R. D. Burkhart
Dept. of Chemistry
Phone: (702)-784-6041
$80,391 03-1

Using pulsed laser excitation and luminescence monitoring in the microsecond time domain, coupled with measurement of ground state depletion, some of the fundamental photophysical rate constants associated with solid films of aromatic polymers at ambient temperature will be studied. The rate constants include those for excimer phosphorescence, radiationless deactivation of long-lived triplet excimers and triplet-triplet annihilation to form delayed excimer fluorescence. Additional investigations in the area of triplet energy transfer from terminal carbonyl groups of polystyrene chains to pendant phenyl groups. The subsequent rates of energy migration along the polymer chain will also be investigated.

NEW MEXICO INSTITUTE OF MINING & TECH.
Socorro, NM 87801

396. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS

O. T. Inal
Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5229, 5519
$95,000 (24 Months) 01-1

Effect of plating geometry, bath compositions and current densities on the surface structure of electroplated black Cr_2O_3 and anodic oxidation of leaf Zn, Zn electroplated steel, and hot-dip galvanized steel. TEM, FIM, nucleation, solar absorption, thermal cycle, mechanical adhesion studies, ZnO and Al_2O_3 film coatings, copper oxide and black nickel selective surfaces, and mathematical optimization of selective solar surfaces.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 87131

397. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE COMPLEX NB-TA-TI OXIDES, PHOSPHATES AND SILICATES

R. C. Ewing
Geology Dept.
Phone: (505)-277-2030
$71,500 01-1

Comparative study of the properties of selected metamict minerals and synthetic irradiated phases of similar compositions. Research includes characterization of changes in properties of crystalline materials as a function of a alpha-recoil dose for natural materials; characterization of the structure of the metamict state in various silicates, phosphates, and oxides using X-ray diffraction, electron microscopy, extended X-ray absorption fine structure and near edge structure (EXAFS/XANES) spectroscopy; determination of kinetics of annealing of natural zircons, pyrochlores and silicate apatites, and complex Nb-Ta-Ti oxides which are partially or completely metamict; and correlation of recrystallization and fission track fading kinetics to predict the role of thermal annealing on long-term radiation effects.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE
New York, NY 10031

398. INVESTIGATIONS OF HARD, CARBON-BASED SURFACE COATINGS: FROM 'DIAMOND-LIKE' CARBON TO SILICON CARBIDE

F. W. Smith
Dept. of Physics
Phone: (212)-690-6963
$93,010 01-1

Preparation of thin-film surface coatings by flow discharge and reactive sputtering of disordered alloys of carbon, silicon, and hydrogen ($C_xSi_yH_z$) with carbon as the primary constituent. Characterization using photoemission, EXAFS, optical spectroscopy (visible and IR) and measurements of density and hardness. Photoemission and carbon K-edge absorption studies using synchroton radiation at the BNL NSLS.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

399. DYNAMICS OF FLUID SURFACES AND THE CRYSTAL-MELT INTERFACE

H. Z. Cummins
Dept. of Physics
Phone: (212)-690-6921

$150,640 (18 Months) 02-2

Study by quasielastic light scattering spectroscopy of two closely related phenomena associated with interfacial dynamics: capillary waves on the free surface of a liquid as a function of temperature, and of the microscopic dynamics of growth - accomplished by investigating the nature of excitations on the interface of a crystal growing into an undercooled melt. To elucidate various aspects of the surface roughening transitions, the genesis of screw dislocations and, ultimately, the morphological instability of a growing crystal surface for dendrite formation.

400. MAGNETIC PROPERTIES OF DOPED SEMICONDUCTORS

M. Sarachik
Dept. of Physics
Phone: (212)-690-6924

$107,000 02-2

A systematic study of the magnetic properties of homogeneous, well-characterized samples of heavily doped semiconductors as a function of impurity concentration across the metal-nonmetal transition. Measurements to be made with a Faraday balance, as a function of temperature (from 1.25 K to 300 K) and of magnetic field (to 50 kG) to separate various contributions to the total susceptibility. Measurements extended to 50 mK and 190 kG at the National Magnet Laboratory. Ascertain whether percolation plays a role in the transition by determining whether a contribution associated with conduction electrons (or holes) persists into the insulating range of concentration.

401. ELECTRONIC AND OPTICAL PROPERTIES OF DISORDERED SYSTEMS

M. Lax
Dept. of Physics
Phone: (212)-690-6864

$91,147 02-3

An extensive theoretical study of transport and optical properties of disordered media such as amorphous materials, doped semiconductors, quasi-one dimensional conductors, interfaces, etc.

STATE UNIVERSITY OF NEW YORK/STONY BROOK
Stony Brook, NY 11794

402. RESEARCH CONSORTIUM FOR X-RAY TOPOGRAPHY ON LINE X-19 AT NSLS

J. C. Bilello
Dept. of Materials Science
Phone: (516)-246-5983

$500,000 01-1

Development of facilities for X-ray topography at the National Synchrotron Light Source (NSLS) and implementation of advanced materials research. Acquisition of image processing equipment and development of associated software for real-time high-resolution data processing. Research includes studies of hydride precipitation in the niobium-hydrogen system, investigations of high temperature grain boundary failure mechanisms, fundamental studies on crack initiation and propagation in elastic-plastic materials, thermal decomposition mechanisms in inorganic single crystals, internal stresses in protective coatings for fusion applications, morphology of CdS after pressure quenching, characterization of strains and effects in metal-silicide thin films on Si substrates and direct measurements of the interaction of acoustic waves in solids with the microstructure.

403. CONSTRUCTION AND MAINTENANCE OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE (SEVERAL INSTITUTIONS INVOLVED)

J. Bigeleisen
Dept. of Chemistry
Phone: (516)-246-7945

$360,000 02-2

An X-ray beam line at the National Synchrotron Light Source (NSLS) developed under the auspices of this Participating Research Team (PRT). This PRT represents campuses at Albany, Buffalo, Stony Brook, Cortland, and Alfred. Facilities and research in high resolution crystallography, surface physics, small angle scattering, and EXAFS.

404. SURFACE STUDIES: A PROPOSAL FOR A PARTICIPATING RESEARCH TEAM AT NSLS

F. Jona
Dept. of Materials Science and Engineering
Phone: (516)-246-7649, 6759

$150,527 02-2

Development of a versatile, high-vacuum experimental chamber for surface research with the VUV ring at NSLS with LEED, Auger, SEXAFS, and photoemission facilities. Studies of atomic structure of solid surfaces: Al, Fe, and Ti, both clean and with O, S, Cl, and CO adsorbates. Chemisorption, physisorption and hydrogen uptake: H uptake by Nb; O on Ni and Nb; Pd on Nb and Ta. Electronic properties of solids: lifetimes of excited states in metals and insulators; effects of bulk phase transitions on surface structure; surface and bulk properties of FeTi.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

405. THEORETICAL STUDIES OF CHEMIADSORPTION ON COPPER-NICKEL ALLOYS AND SURFACE EMBRITTLEMENT

J. L. Whitten
Dept. of Chemistry
Phone: (516)-246-6068

$100,000 03-3

A recently developed embedding theory for treating chemisorption on metals extended and applied to systems involving titanium, copper, nickel and copper/nickel alloy substrates, and H_2, H, CO, C and coabsorbed H and C adsorbates. Two of the studies, surface embrittlement of titanium by hydrogen and H_2 dissociation on a monolayer stepped copper surface are extensions of previous work. The major copper/nickel alloy project is a systematic variation of the surface composition by Cu/Ni substitution in order to probe the effect of surface composition on H and CO adsorption and the nature of the carbon-metal bond. The primary emphasis of the work is on the energetics of adsorption as a function of surface composition, with the objective of determining the reactivity of adsorbed species.

NORTH CAROLINA AGRICULTURAL & TECH. UNIVERSITY
Greensboro, NC 27411

406. EFFECT OF THERMAL AND CYCLIC LOADS ON SILICON CARBIDE YARN REINFORCED GLASS MATRIX COMPOSITES

V. S. Avva
Dept. of Mechanical Engineering
Phone: (919)-379-7620
J. Sankar
Dept. of Mechanical Engineering
Phone: (919)-379-7620

$60,000 01-5

Characterization of SiC/glass matrix fibers before, during, and after tension-tension and thermal fatigue testing from room temperature to 600°C at a stress amplitude ratio of 0.1 and a frequency of 10Hz. Radiographic examination for delamination, debonding, fiber breakage, etc. Optical and scanning electron microstructural characterization.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27650

407. MICROSTRUCTURAL EFFECTS IN SOLID PARTICLE EROSION

H. Conrad
Dept. of Materials Engineering
Phone: (919)-737-2377
R. O. Scattergood
Dept. of Materials Engineering
Phone: (919)-737-2377

$90,350 01-5

Correlation of erosion rates in multiphase systems with constituent phase properties and distribution. Systems under investigation: Al-Si alloys, WC-Co cermets and alumina-stainless steel composites. Systematic measurement of erosion rates as a function of operational variables (particle size, velocity angle-of-incidence) and microstructural variables (volume fraction, phase size and distribution, alloy content). SEM observations on steady-state erosion surfaces and single impact events. Constituitive and averaging laws for erosion rates to be developed from experimental results and modeling/computer simulation.

NORTH CAROLINA CENTRAL UNIVERSITY
Durham, NC 27707

408. VIBRATIONAL PROPERTIES OF DISORDERED SOLIDS: FAR INFRARED STUDIES

J. M. Dutta
Dept. of Physics
Phone: (919)-683-6452
C. R. Jones
Dept. of Physics
Phone: (919)-683-6452

$65,843 02-2

Measurements of low-frequency vibrational properties of disordered solids in the far infrared region (5 cm^{-1} to 150 cm^{-1}) as a function of temperature using laser techniques. Materials studied: various forms of quartz and fused silica, alumina and magnesia. Other materials of interest: BeO, BN, and Si_3N_4. Effects on dielectric properties due to the presence and concentration of impurities and sintering acids, and to microstructural properties, investigated in selected materials. Experimental data compared with existing theoretical models.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27650

409. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY (PRT)

D. E. Sayers
Dept. of Physics
Phone: (919)-737-2512

$240,000 02-2

Development of an advanced X-ray absorption fine structure (EXAFS) beam line at NSLS for a Participating Research Team (PRT) with members from North Carolina State University, University of Connecticut, University of Washington, University of Delaware, Brookhaven National Laboratory, United Technologies and General Electric. Facility for the energy range from 1-20 KeV and with provisions for EXAFS, fluorescence, and near edge spectroscopic and polarization studies. Research to be addressed: areas of metallurgy, corrosion, amorphous materials, catalysis, interfacial phenomena, electrochemistry and magnetic properties.

NORTHEASTERN UNIVERSITY
Boston, MA 02115

410. DYNAMICAL FRICTION IN CONDENSED MATTER

J. B. Sokoloff
Dept. of Physics
Phone: (617)-437-2931
C. H. Perry
Dept. of Physics
Phone: (617)-437-2913

$89,996 02-3

Joint theoretical-experimental studies of a variety of systems reflecting motion of one set of species (ions, defects, layers) relative to another set of species (channels, lattices, layers). The rate of energy dissipation, its frequency, temperature and pressure dependence will be calculated as well as electronic contributions to the damping. Experimental studies of Y_2O_3 - ZrO_2, hollandite perovskite, intercalated graphite and dichalcogenides will be related to the theoretical models, including a predicted electric field effect.

NORTHWESTERN UNIVERSITY
Evanston, IL 60201

411. POINT DEFECT CLUSTERS AND ELECTRICAL BEHAVIOR IN TRANSITION METAL OXIDES

J. B. Cohen
Dept. of Materials Science and Engineering
Phone: (312)-492-3570
D. E. Ellis
Dept. of Physics and Astronomy
Phone: (312)-492-3665
T. O. Mason
Dept. of Materials Science and Engineering
Phone: (312)-492-3198

$175,525 01-1

Interdisciplinary study of the first row transition metal monoxides, combining measurements of defect structure and electrical properties with quantum theoretical calculations. These oxides represent a "model" series which, while sharing the average structure of NaCl, exhibit a wide range of stoichiometries, defect structures, and conduction mechanisms. Electrical measurements and conduction mechanism analysis extended to MnO and NiO. Valence in the series will be studied via X-ray absorption edge, T.E.M. critical voltage technique, and photoelectron spectroscopy. Defect interactions in MnO and CoO studied via X-ray (synchrotron) and/or pulsed neutron scattering. The self-consistent field local density theory used to calculate the electronic structure associated with isolated vacancies and defect clusters. An energy band code based on the Linearized Muffin Tin scheme used to calculate band structures, Fermi surfaces, and transport properties to correlate with the experimental studies. Theory made to more complex oxides, e.g., Fe_3O_4, $CoAl_2O_4$, and $FeAl_2O_4$.

412. FAST ION MOTION IN SELECTED VITREOUS AND CRYSTALLINE SOLID ELECTROLYTES

D. H. Whitmore
Dept. of Materials Science and Engineering
Phone: (312)-492-3533

$74,946 01-1

Diffusivity of highly mobile ions in solid electrolytes which may have application in energy storage or conversion is measured using pulsed-field-gradient nuclear magnetic resonance techniques and analyzed using a dynamic bond percolation model. Specific materials to be studied include protonic-conducting crystalline beta-alumina and gallates and fast-ion conducting glasses.

NORTHWESTERN UNIVERSITY (continued)

413. AN INVESTIGATION OF MICROSTRUCTURAL CHANGES IN FERRITIC STAINLESS STEELS CAUSED BY HIGH TEMPERATURE DEFORMATION

J. R. Weertman
Dept. of Materials Science and Engineering
Phone: (312)-492-5353
$65,100 01-2

Investigation of deformation, failure, and microstructural stability during creep and creep fatigue in ferritic stainless steels; influence of thermal and mechanical history, environment, and alloy composition on mechanical properties; HVEM and SANS characterization of strain and thermal induced microstructural modifications. e.g., carbide precipitation, dislocation structures, cavity formation.

414. PRODUCTION AND STUDY OF NEW MATERIALS USING CLUSTER BEAMS

G. D. Stein
Depts. of Materials Sci. & Eng., and Mechanical & Nuclear Eng.
Phone: (312)-492-3263
$114,996 01-3

Experimental and theoretical research on: a) the development of new metal cluster sources, including binary alloy clusters, b) the comparison of cluster properties in low density molecular beams to those of the same species collected onto substrates or in matrix isolation, and c) the production of new composite materials using cluster deposition. High energy electron diffraction and laser scattering are used to study the structures and the onset of nucleation of metallic clusters as small ten atoms per cluster. These studies are carried out on clusters in-flight prior to deposition onto substrates; clusters as small as fifty atoms per cluster have been studied to date.

415. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMICONDUCTING ZINC SULPHO-SELENIDE

B. W. Wessels
Dept. of Materials Science and Engineering
Phone: (312)-492-3219
$64,395 (15 Months) 01-3

Investigation of fundamental point defect formation mechanisms in the wide bandgap semiconductor ZnSSe. Identification of deep level defects in deliberately doped and MeV electron irradiated material and exploration of their role in electrical compensation. Thermal stability of defects. Experimental techniques include optical and electrical deep level transients spectroscopy, Hall measurements, photocapacitance, and spectrally resolved photocurrent measurements.

NORTHWESTERN UNIVERSITY (continued)

416. ULTRA-LOW-TEMPERATURE NEUTRON DIFFRACTION

W. P. Halperin
Dept. of Physics and Astronomy
Phone: (312)-492-3686, 3644
J. B. Ketterson
Dept. of Physics and Astronomy
Phone: (312)-492-5468, 3644

$110,000 (24 Months) 02-1

Investigations of nuclear magnetic ordering using an ultralow temperature neutron diffraction facility at Argonne National Laboratory. Determination of the nature of the nuclear ordering in solid helium-3, a result of fundamental importance. Investigation of the ordering of nuclear spins in metals such as $PrCu_6$.

417. LOCAL DENSITY THEORY OF HEATS OF FORMATION AND SHORT-RANGE-ORDER PARAMETERS IN SUBSTITUTIONALLY DISORDERED ALLOYS

A. J. Freeman
Dept. of Physics and Astronomy
Phone: (312)-492-3685, 3644
A. Gonis
Dept. of Physics and Astronomy

$70,000 02-3

Determination of the thermodynamic properties and short-range order(SRO) parameters of ordered and substitutionally disordered alloys from ab-initio all-electron calculations taking into account the lattice structure, statistical fluctuations and utilizing fully relativistic energy band programs. Recently developed theoretical and computational methods based on local density theory and a cluster generalization of the coherent potential approximation (CPA) used to obtain the density of states. These calculations to identify multi-site potentials to be used with existing theories, such as the cluster variation method of Kikuchi, to construct alloy phase diagrams.

NORTHWESTERN UNIVERSITY (Coninued)

418. STUDIES OF THE SHEAR RESPONSE AND STRUCTURE OF MONOMOLECULAR FILMS ON THE SURFACE OF WATER

P. Dutta
Dept. of Physics and Astronomy
Phone: (312)-492-5465
J. B. Ketterson
Dept. of Physics and Astronomy
Phone: (312)-492-3644

$97,809 03-3

Study of the mechanical properties of organic monolayers on the surface of water (Langumuir films). The microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) studied using X-rays and ellipsometry. Studies of the mechanical properties directed toward the shear response, an important but previously neglected structural property. A diffraction technique involving external reflection at the monolayer surface used to determine structure. Finally the loss of certain symmetry elements of surface phases studied by observing the rotation of plane polarized light incident normal to the surface. A search for this effect within the so-called liquid expanded-liquid-condensed region, which may be a liquid crystal phase.

UNIVERSITY OF NOTRE DAME
Notre Dame, IN 46556

419. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR

T. H. Kosel
Dept. of Metallurgical Engineering and Materials Science
Phone: (219)-239-5642

$84,700 01-5

Assessment of mechanisms controlling abrasive wear in multiphase Fe- and Co-base alloys; influence of second phase particle toughness, size and volume fraction; changes in near-surface microstructure during abrasion; influence of abrasive size, hardness, angularity and loading conditions; in situ SEM scratch test simulations of fixed-abrasive abrasion mechanisms.

OHIO STATE UNIVERSITY
Columbus, OH 43210

420. INFLUENCE OF NITROGEN ON THE SENSITIZATION, CORROSION, MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF AUSTENITIC STAINLESS STEELS

W. A. T. Clark
Dept. of Metallurgical Engineering
Phone: (614)-422-2538
B. Wilde
Dept. of Metallurgical Engineering
Phone: (614)-422-6255
D. D. Macdonald
Chemistry Lab, SRI International
Phone: (415)-859-3195

$75,000 01-1

Evaluation of corrosion and stress corrosion cracking of austenitic stainless steel with various C and N contents; TEM characterization of grain boundary structure as well as carbide and nitride morphologies, compositions, and distributions; measurement of electrochemical parameters in static and flowing aqueous solutions containing chloride and sulphate ions.

421. GENERATION OF MICROPOROSITY IN STEEL WELDS AND ITS ROLE IN HYDROGEN ATTACK

P. G. Shewmon
Dept. of Metallurgical Engineering
Phone: (614)-422-2491

$65,992 01-2

Investigation of mechanisms controlling hydrogen attack in bainitic steels, with emphasis on evaluating degradation in weldments made by various processes -- gas tungsten and submerged arc welding as well as electroslag welding; characterization of microporosity with electron microscopy (both TEM and SEM) and dilatometry, respectively, to indicate the microstructural features where attack initiates and the overall kinetics of attack; assessment of role of matrix creep and of susceptibility of fusion vs. heat affected zone to attack.

422. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

R. A. Rapp
Dept. of Metallurgical Engineering
Phone: (614)-422-6178

$99,950 01-3

In-situ SEM study of oxidation of metals, Fe, Ni, Cu and Cr, and binary alloys of these metals; effect of H_2 on oxide morphology; influence of surface treatment on oxidation of Cr; pore development at metal-scale interface; oxide morphologies, e.g., pits and ledges in Fe_2O_3 and whiskers in NiO.

OHIO STATE UNIVERSITY (continued)

423. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT BOUNDARIES SEPARATING ANISOTROPIC MATERIALS

L. Adler
Dept. of Welding Engineering
Phone: (614)-422-1974
$111,245 01-5

Experimental and analytical research to study interactions of ultrasonic waves with boundaries separating anisotropic materials. Single crystals of nickel prepared and diffusion bonded to both polycrystalline and other single crystals. Computer controlled ultrasonic parameters in the crystals and at the boundaries. Analysis of energy transport and wave partitioning

PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

424. PHYSICAL CHEMISTRY OF PORTLAND-CEMENT HYDRATE, RADIOACTIVE WASTE-HOSTS

M. W. Grutzeck
Materials Research Laboratory
Phone: (814)-865-3539
$59,817 01-1

Physical and crystal chemistry of three portland-cement hydrates: calcium silicate hydrates, calcium aluminum hydrates, and calcium alumino silicate hydrates. Phase-equilibrium relationships governing the hydration of portland cement, both with and without radioactive waste. Fixation of iodine by calcium aluminate hydrates and the feasibility of using Stratling's compound and its associated hydrates as host phases for cesium and strontium fixation. Identification fo phases best suited for hosting selected radioactive-waste ions, and synthesis and crystallographic characterization of such phases. Solubility/leachability study of synthesized host phases both individually and encapsulated in a suitable cementitious matrix.

PENNSYLVANIA STATE UNIVERSITY (continued)

425. VIBRATIONAL AND OPTICAL STUDIES OF AMORPHOUS METALS

J. S. Lannin
Dept. of Physics
Phone: (814)-865-9231

$82,800 01-1

Research aimed at developing the method of interference enhanced Raman scattering (IERS) to study the structure, bonding, and stability of amorphous metal alloys. The basis of the IERS technique is to fabricate thin film trilayer structures of the materials to be studied which include dielectric layer and reflecting layer to produce a minimum in the reflectance and thus reduce the background light when measuring the Raman scattered light. The study is initially focussed on metalloid alloys and will subsequently be extended to amorphous metals in general. Complementary inelastic neutron scattering measurements are also employed for structure, bonding and short-range order determinations.

426. SPECTROSCOPIC INVESTIGATIONS OF GLASS STRUCTURE

W. B. White
Materials Research Laboratory
Phone: (814)-865-1152

$116,881 01-1

Glasses containing transition metal ions are studied utilizing Raman, infrared, optical absorption, and luminescence spectroscopy. Specific investigations include (i) the local environment of alkali ions in silicate glasses by far infared spectroscopy, (ii) processes of phase separations as related to heat treatment by high-temperature Raman spectroscopy, (iii) the relationship of Raman spectra to thermodynamic quantities in silicate glasses, (iv) formation of transition metal complexes in glass, and (v) clustering and nucleation of transition metals in high magnesium content glasses.

427. GRAIN BOUNDARY AND SURFACE DIFFUSION IN OXIDE SYSTEMS

V. S. Stubican
Dept. of Materials Science
Phone: (814)-865-9921

$54,800 01-3

Grain boundary impurity diffusion in ionic materials, specifically isotopes of Cr and Fe in Fe_3O_4; influence of point defects on the grain boundary diffusion. Chemistry of grain boundaries. Surface diffusion in oxide materials, specifically isotope of Cr on surfaces of MgO, Al_2O_3, and NiO or isotopes of Cr and Co on CoO surface. Chemistry of surfaces. Techniques used: gamma-rays counting, SIMS, Auger, LEED.

PENNSYLVANIA STATE UNIVERSITY (continued)

428. EXPERIMENTAL AND THEORETICAL STUDIES ON TRANSPORT PROCESSES IN LASER WELDING

T. DebRoy
Dept. of Materials Science and Engineering
Phone: (814)-865-1974

$64,516 01-5

Modelling of solute loss, heat transfer and fluid flow during laser welding of stainless steels. Calculation of local temperature profile, weld pool velocity and vaporization of alloying elements; correlative experimental determination of weld microstructure and chemistry; time resolved emission spectroscopic measurements to determine composition of metal vapors.

429. MECHANISMS OF WEAR IN SINGLE AND TWO PHASE MATERIALS

N. H. Macmillan
Materials Research Laboratory
Phone: (814)-863-0180

$96,200 01-5

Experimental comparison of the resistance of various classes of materials to solid particle erosion, slurry erosion, and rolling-tumbling-sliding wear by angular WC-Co particles; specimen preparation by powder methods; study of particle trajectories and impact parameters by cinematography; characterization of wear by optical and electron microscopy, weight loss measurements and surface profilometry. Materials systems to include (i) brittle ($PbO-B_2O_3-SiO_2$ glass, Al_2O_3) and ductile (Pb,Cu) single phase and (ii) brittle-brittle (Al_2O_3 in $PbO-B_2O_3-SiO_2$ glass), brittle-ductile (Al_2O_3 in Pb), ductile-brittle (Cu in $PbO-B_2O_3-SiO_2$ glass) and ductile-ductile diphasic materials.

430. LASER PROCESSING OF CERAMICS

G. L. Messing
Dept. of Materials Science and Engineering
Phone: (814)-865-2262

$63,000 01-5

Correlations between melt crystallization kinetics, thermodynamics, phase equilibria, etc. during rapid solidification of $Al_2O_3-SiO_2$ compositions around the mullite phase field and $Al_2O_3-ZrO_2$ both melted with a 10.6 micron CO_2 laser. Preparation of ceramic powders using rapid solidification processing by injecting solutions and/or solid particles coaxially into a plasma flame. Investigation of morphological modification by single particle melting and rapid solidification, calcination of oxide precursors and rapid reaction of multicomponent systems. Formation and properties of mullite powders with respect to phase equilibria, plasma parameters, and solidification conditions.

PENNSYLVANIA STATE UNIVERSITY (continued)

431. STUDY OF FIELD ADSORPTION USING IMAGING ATOM-PROBE ION MICROSCOPY

T. T. Tsong
Dept. of Physics
Phone: (814)-865-2813
$88,000 02-2

Study in atomic detail of field adsorption of noble gases and classical molecular gases using the imaging atom probe field ion microscope. Measurement of adsorption energy as a function of field on catalytically active group VIII metal surfaces. Mechanism of formation of metal-noble gas complex ions. Photon and electron stimulated field desorption.

UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

432. ATOMISTIC STUDIES OF THE STRUCTURAL PROPERTIES OF GRAIN BOUNDARIES WITH SUBSTITUTIONAL IMPURITIES

V. Vitek
Dept. of Materials Science and Engineering
Phone: (215)-898-7883
$79,973 01-1

Atomistic computer simulation studies of the structure and properties of grain boundaries containing various concentrations of alloying element; the alloys considered are Cu-Bi, Au-Ag, Cu-Ag, Fe-Sb, Fe-Cu, Fe-Sn. Development of semiempirical scheme for description of interatomic forces in pure metals and alloys in the form of pair potentials and volume dependent term by fitting elastic properties, lattice parameter, cohesive energy, enthalpy of mixing and charge transfers. Relationship between grain boundary structure and propensity to segregation; structural transformations induced by segregation and influence on diffusion, emission and absorption of vacancies and boundary migration; trapping of hydrogen and helium in grain boundaries and their effect on embrittlement.

UNIVERSITY OF PENNSYLVANIA (continued)

433. LOW STRESS BRITTLE FRACTURE IN POLYMERS

N. Brown
Dept. of Materials Science and Engineering
Phone: (215)-898-8506

$81,500	01-2

Initiation of slow crack growth in polyethylene, ethyleneoctene copolymers with various octene concentrations branch densities of 2-10 per 100 carbon atoms and narrow molecular weight distribution. Measurement under plane strain of rate of formation of damaged zone at root of a notch as function of stress, time, temperature, notch depth, specimen geometry. Characterization of extent of porous, fibrillated and fractured regions which constitute the damaged zone using optical microscopy, SEM and TEM. Determination of constitutive equations for various regions of damaged zone. Use of data to construct a mathematical model based on the micro-mechanics of fracture for predicting long time failure in engineering structures.

434. MECHANISMS OF DAMAGE ACCUMULATION IN TIME-DEPENDENT CYCLIC DEFORMATION

C. Laird
Dept. of Materials Science and Engineering
Phone: (215)-898-8337
J. Bassani
Dept. of Mech. Eng. and App. Mechs.
Phone: (215)-898-5632

$106,000	01-2

Identification of microsctructural changes resulting from cyclic creep and fatigue deformation of metals, initially Cu and Cr-Mo-V steel; relationship of developing embrittlement of fatigue-induced compositional changes in carbides (Cr-Mo-V); mechanisms of failure in fatigue loading with and without mean loads and its relationships with microstructure; modelling of fatigue-induced property changes; cyclic stress-strain response in the presence of mean loads and its relation to fracture; behavior of single crystals in cyclic creep with special reference to latent hardening; development of effective numerical techniques to model single crystal plasticity by slip; modelling of polycrystalline behavior.

UNIVERSITY OF PENNSYLVANIA (continued)

435. INTRINSIC SURFACE PHONONS ON RECONSTRUCTED SEMICONDUCTOR SURFACES

E. J. Mele
Dept. of Physics
Phone: (215)-898-3135

$104,216 02-3

Theoretical study of the lattice dynamics of reconstructed semiconductor surfaces. Relation between localized surface electronic and surface structural and vibrational properties. Computation scheme combines a short range elastic Hamiltonian with a static electronic polarization extracted from a tight binding representation of the valence electronic bands. Applications include models of Si(100)2x1 and Si(111)2x1 surfaces and generalization of the results to deduce a structural Hamiltonian for Ge.

436. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES

G. C. Farrington
Dept. of Materials Science and Engineering
Phone: (215)-898-6642

$103,127 03-1

Preparation and characterization of a series of solid state protonic conductors, for use in the temperature range of 100-400°C. Determination of conductivities of NH_4^+-H^+- aluminas, and studies of the influence of the stabilizing cation. Studies on single crystals of deuteronium beta and beta" alumina including refinements of atomic positions, band lengths, etc. NMR studies to explore microscopic processes of diffusion.

UNIVERSITY OF PITTSBURGH
Pittsburgh, PA 15261

437. HIGH TEMPERATURE CORROSION OF CERAMICS

F. S. Pettit
Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5300
J. R. Blachere
Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5296

$65,000 01-3

Thermodynamic and kinetic analyses of gaseous and molten salt corrosion of oxides (SiO_2, Al_2O_3, Cr_2O_3, and ZrO_2) in oxidizing, sulfidizing, and reducing environments; thermogravimetric measurement of corrosion kinetics. Gas mixtures of SO_2-SO_3-O_2, H_2-H_2O, and CO-CO_2-O_2 at temperatures in the interval 700° to 1400°C. Effects of deposits such as Na_2SO_4, NaOH and Na_2CO_3 on the gas-induced corrosion. Mechanisms of corrosion of high purity materials and of materials with microstructures and impurities characteristic of advanced commercial materials. Morphology of the corrosion products.

UNIVERSITY OF PITTSBURGH (continued)

438. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES

J. V. Maher
Dept. of Physics and Astronomy
Phone: (412)-624-0872

$115,300 (15 Months) 02-2

Studies of the physics of binary liquid interfaces. Experiments on onset and nonlinear growth of hydrodynamic instabilities, nonlinear pattern formation, and transition to turbulence. The diffusion-driven instability of a quenched liquid interface and the Saffman-Taylor instability (viscous fingering) investigated with careful control over such parameters as density difference, viscosity difference, and interfacial tension. Light scattering investigations of the dynamics of phase separation for a binary liquid mixture imprisoned in a gel to understand the role of hydrodynamics.

POLYTECHNIC INSTITUTE OF NEW YORK
333 Jay Street
Brooklyn, NY 11201

439. PHOTOEMISSION STUDIES OF F-ELECTRON SYSTEMS: MANY BODY EFFECTS

R. D. Parks
Dept. of Physics
Phone: (212)-643-2071

$90,000 02-2

Photoemission studies of rare earth and early actinide systems with the aim of understanding the electronic phenomena underlying the 4f-instabilities in mixed valent and Kondo lattice systems and narrow 5f-band behavior in the early actinides. XPS studies performed at Polytechnic and synchrotron-radiation-stimulated photoemission studies at NSLS.

440. MIXED VALENT BEHAVIOR IN ACTINIDES AND RELATIONSHIP TO CERIUM

P. S. Riseborough
Dept. of Physics
Phone: (212)-643-5011

$106,667 (18 Months) 02-3

Theoretical research on the many body aspects of materials containing the early actinide elements and Ce. Principal subjects: the direct relationships between the magnetic properties, conduction electron-spin scattering effects in transport properties, and the single particle excitation spectrum as seen in photoemission and Bremsstrahlung isochromat spectroscopies. The basic theoretical model: a lattice of magnetic ions (Anderson lattice) in which the magnetic f electrons can be delocalized by both the direct f-f overlap and the hybridization with the valence band. The role of electron phonon-mediated couplings and other possible exotic coupling mechanisms in the heavy fermion superconductors $CeCu_2Si_2$, UBe_{13} and UPt_3.

POLYTECHNIC INSTITUTE OF NEW YORK (continued)

441. LOCAL MANY-BODY EFFECTS IN THE OPTICAL RESPONSE OF NARROW BAND SOLIDS

A. Zangwill
Dept. of Physics
Phone: (212)-643-2190
D. Liberman
Lawrence Livermore National Laboratory
$57,613 (16 Months) 02-3

Provide realistic calculations of expected photoelectric partial cross sections for the late 3d transition metals, cerium, the light actinides and the associated intermetallic compounds of all the aforementioned. Such calculations to provide essential guidance in interpretation of experiments involving photoabsorption and photoemission measurements in the vicinity of near core and deep core thresholds. Calculation from RPA-type theory based on the density functional formalism applied to an embedded cluster model of condensed matter. Special care will be taken to simulate the interplay between dielectric and core-hole many-body effects, both of which are expected to be important in the materials of interest.

PRINCETON UNIVERSITY
Princeton, NJ 08544

442. MODULATED INFRARED LINEAR DICHROISM STUDIES OF THE DYNAMICS OF MOLECULAR ORIENTATION AND RELAXATION IN POLYMERS

J. T. Koberstein
Dept. of Chemical Engineering
Phone: (609)-452-5721
R. K. Prud'homme
Dept. of Chemical Engineering
Phone: (609)-452-4577
$80,000 03-1

A program is proposed to examine the fundamental relationship between chain conformational changes and resultant macroscopic material responses during deformation. The program is based on the coupling of rheological and rheo-optical measurements during deformation. An in situ infrared dichroism technique is described by which molecular orientation may be characterized dynamically during polymer deformation and relaxation. The use of novel specimens that are partially deuterium labelled allows characterization of local chain segment orientation. The information is not obtainable by present techniques and is of sufficient detail to allow a test of current theories of polymer chain relaxation by reputational motion. The information is of importance in understanding the relationship between polymer processing conditions and polymer material behavior.

PRINCETON UNIVERSITY (continued)

443. ASPECTS OF PHOTOIONIZATION OF IMPURITIES AND ELECTRON TRANSFER IN IONIC CRYSTALS

D. S. McClure
Dept. of Chemistry
Phone: (609)-452-4980

$85,000	03-1

Research is proposed on the relationship between the energy levels of impurity ions and the energy levels in the host crystal. The method to be used is measurement of photoionization thresholds of the impurity ions. Included is research of the process of electron ejection into the lattice by studying the phototransfer of electrons from a set of donor ions to a set of acceptor ions. Related research on the local geometry of the crystal in the vicinity of the ion which have lost an electron and the formation of exciplexes is also proposed.

PURDUE UNIVERSITY
West Lafayette, IN 47907

444. NOVEL POLYMERIC Li AND DIVALENT CATION FAST ION CONDUCTING MATERIALS: LI-SALT-IONENIC POLYMER SOLUTIONS, LI CONTAINING PLASTIC CRYSTAL PHASES AND MI_2-$M(PO_3)_2M(PS_3)_2$ GLASSES

C. A. Angell
Dept. of Chemistry
Phone: (317)-494-5256
E. I. Cooper
Dept. of Chemistry
Phone: (317)-494-5256

$82,782	01-1

Preparation and characterization of novel fast ion conductors. Formation of a unique type of "molten salt" systems by dissolution of lithium salts in salts of quaternary nitrogen cations in eight polymeric or related structure forms. Studies of Li^+-ion conduction mechanisms. Examination of the possibility of obtaining glasses with a relatively high conductivity in which the charge carrier is a divalent cation. Target systems include MI_2-$M(PO_3)_2M(PS_3)_2$, where M^{2+} is Pb^{2+}, Cd^{2+}. Characterizations include measurements of electrical conductivity, nuclear magnetic resonance, vicsoelastic properties, and glass transition temperatures.

PURDUE UNIVERSITY (continued)

445. INSTRUMENTATION OF X-RAY DIFFRACTION AND MATERIALS RESEARCH ON THE NATIONAL SYNCHROTRON LIGHT SOURCE

G. L. Liedl
School of Materials Engineering
Phone: (317)-494-4095

$480,000 01-1

Development and operation of a high intensity X-ray synchrotron beam line for X-ray diffraction studies involving scientists primarily from midwestern institutions (principal institutions are University of Illinois, Northwestern University, Purdue University, Iowa State University, University of Missouri, and Argonne National Laboratory). Major research efforts on phase transformation studies and X-ray surface diffraction, with specific topics including: substitutional solutes in FCC systems, interstitial solutes, clustering of vacancies in oxides, martensitic transformations non-equilibrium phonons in crystals, phase transitions in 2D systems, structure of small iron particles, structure of organic layers, melting of grain and phase boundaries, electronic materials interfaces, and heterogeneous catalysis.

446. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

A. A. Solomon
School of Nuclear Engineering
Phone: (317)-494-5753

$93,000 01-2

Study of elevated temperature tensile creep and stress rupture in well-characterized single phase ceramics in terms of rate controlling mechanisms and microstructural evolution. Experimental techniques consist of (a) tensile creep using constant true stress, (b) internal pressurization of pores with inert insoluble gas and microscopic measurement of pore or cavity growth under known hydrostatic pressure and surface tension driving forces. Results are correlated with quantitative microstructural studies of porosity evolution. Materials under investigation are CoO, UO_2, NiO and carbonyl Ni.

PURDUE UNIVERSITY (continued)

447. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT DIFFUSION

M. A. Dayananda
School of Materials Engineering
Phone: (317)-494-4113
$87,917 01-3

The objectives are (a) to explore the role and development of zero-flux planes (ZFP) and flux reversals in both single phase and multiphase diffusion couples in multicomponent systems during isothermal diffusion; (b) to characterize the ZFP compositions in terms of diffusion paths and thermodynamic data; (c) to study the feasibility of regulating the interdiffusion of elements with preferential development of ZFP's. ZFP's for individual components within the diffusion zone of either a single or multiphase multicomponent have been identified. At ZFP's the interdiffusion flux of a given component goes to zero and exhibits reversal in its flow direction on either side of the plane.

448. STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA

H. Sato
School of Materials Engineering
Phone: (317)-494-4096
R. Kikuchi
School of Materials Engineering
Phone: (317)-494-4099
$89,119 01-3

Research on multicomponent diffusion under general chemical potential gradients. Application of the path probability method of irreversible statistical mechanics to analytically derive the Onsager relations for diffusion on an atomistic basis. The conditions treated are general enabling relations among measurable quantities under a variety of driving forces such as the Nernst-Einstein relation and the Haven ratio in multicomponent systems, to the be clearly understood. The general formalism of multicomponent diffusion and cross terms in the Onsager relations is examined, and the role of apparent vacancy flows and "wind" effects investigated. The method is applied to chemical diffusion problems in multicomponent systems and to understanding established empirical concepts such as "diffusion path" and "zero flux planes."

PURDUE UNIVERSITY (continued)

449. A STUDY OF THE INTERACTION OF LIGHT WITH SUB-MICRON METALLIC SURFACES

R. G. Reifenberger
Dept. of Physics
Phone: (317)-494-3032

$100,000 (18 Months) 02-2

Measurements to provide quantitative information about the interaction of laser light in the visible and near ultraviolet with metallic surfaces of sub-micron extent. Studies of the photo-excitation and subsequent emission of electrons at energies below threshold through the surface potential barrier, the thermal effects associated with the illumination of the surface, and the laser-induced diffusion of adsorbates over the sub-micron surface.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, NY 12181

450. TESTS AND MODELING FOR SINTERING THEORY

R. H. Doremus
Dept. of Materials Engineering
Phone: (518)-266-6709
R. M. German
Dept. of Materials Engineering
Phone: (518)-266-6445

$85,000 01-1

Critical assessment of sintering theories. Measurements of particle, grain, and pore size and shape, shrinkage, surface area, and neck size during the sintering of sodium chloride, aluminum oxide, and aluminum-chromium oxide. Measurements and experimental techniques include dilatometry, buoyancy for density, scanning and transmission electron microscopy, X-ray line broadening, mercury porisometry, and BET surface adsorption.

451. EFFECT OF WELDING VARIABLES ON THE SOLIDIFICATION SUBSTRUCTURE, MECHANICAL PROPERTIES & CORROSION BEHAVIOR OF STAINLESS STEEL

W. F. Savage
Materials Division
Phone: (518)-266-6780
D. J. Duquette
Materials Division
Phone: (518)-266-6490

$141,875 01-1

Corrosion of ferritic steel weldments in aqueous chloride environments; and the effect of welding parameters; effect of delta ferrite on localized corrosion; Cr depletion at grain boundaries; synergistic effect of sulfate and chloride ions on initiation and propagation of stress corrosion cracks; role of grain boundary precipitation; role of surface films; weldability and hot cracking of ferritic steels.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

452. OXIDATION MECHANISMS IN METALS

R. K. MacCrone
Dept. of Materials Engineering
Phone: (518)-266-6047

$80,000 01-3

Study of both point defects, impurities, and grain boundaries in films of the metal oxides NiO, WO_2. Techniques include both discontinuous and continuous thermogravimetric analysis, electron paramagnetic resonance, Raman spectroscopy, TEM, static magnetization, and two point electrical conductivity for the purpose of obtaining a more precise understanding of the oxidation process.

453. PHOTON SCATTERING AND INTERACTION ANALYSIS OF INTERFACIAL CORROSION AND CATALYSIS

T. E. Furtak
Dept. of Physics
Phone: (518)-266-6454

$145,704 02-2

Fundamental problems associated with electrochemical corrosion and catalysis studied through microscopic specification of the structure, energetics, and kinetics of the solid-liquid interface. Non-traditional optical techniques developed and exploited: Raman spectroscopy, reflectance and ellipsometry, photovoltage spectroscopy, infrared emission, and X-ray absorption fine structure.

RESEARCH INSTITUTE OF COLORADO
Condensed Matter Laboratory
Fort Collins, CO 80526

454. PROPERTIES OF MOLECULAR SOLIDS AT HIGH PRESSURE AND TEMPERATURE

R. D. Etters
Dept. of Physics
Phone: (303)-491-5374

$66,773 02-3

Calculations by various techniques of the properties of classes of molecular solids over ranges of temperature and pressure. Properties of interest: equation of state, pressure dependence of lattice vibrational and librational modes, structural and orientational phase transitions, energy transfer mechanisms, virial coefficients, viscosities transport properties, combustion and detonation phenomena and synthesis of new materials.

RICE UNIVERSITY
P. O. Box 1892
Houston, TX 77251

455. STUDY OF THE KINETICS AND THERMODYNAMICS OF HYDROGEN IN PD-BASED ALLOYS

R. B. McLellan
Dept. of Mechanical Engineering and Materials Science
Phone: (713)-527-4993

$54,955 01-3

Systematic measurements of the solubility, thermodynamic properties, and diffusivity of H atoms in the same Pd-based binary alloys. Low (270-350K) and high (500-1000K) temperature diffusion measurements respectively by a double-cell electrolyte system and the permeability time-lag method. Measurement of the temperature and pressure dependence of hydrogen solubility and the temperature and the substitutional solute concentration dependence of the elastic constants. Magnetic susceptibility and elastic constant measurements for Pd and Pd alloys. Statistical thermodynamic modelling. Theoretical models based upon Thiele moment expansions and cell cluster techniques for interstitial solid solutions containing secondary defects (e.g., vacancies).

456. ELECTRON SPIN POLARIZATION EFFECTS IN LEED ION NEUTRALIZATION AND METASTABLE ATOM DEEXCITATION AT SOLID SURFACES

G. K. Walters
Dept. of Physics
Phone: (713)-527-4937
F. B. Dunning
Dept. of Physics
Phone: (713)-527-8101

$185,000 02-2

Polarized Low Energy Electron Diffraction, (PLEED) study of absorption systems: e.g., Ni with Te adsorbed and W with H absorbed. Spin polarization measurements in conjunction with ion neutralization spectroscopy (INS) and metastable deexcitation spectroscopy (MDS) to study surface electronic structure on magnetic materials such as Ni. Polarized He^+ beams used for INS and polarized $He(2^3S)$ beams for MDS.

UNIVERSITY OF ROCHESTER
Rochester, NY 14627

457. FRACTURE TOUGHNESS OF MATERIALS

S. J. Burns
Dept. of Mechanical Engineering
Phone: (716)-275-4082

$90,000 01-2

Research on the relationships between deformation processes and phase transformations occurring at the tips of cracks and the fracture toughness of materials. Specific activities include observations of deformation structures at the tips of cracks in single crystals of LiF and Si, analysis of dislocation nucleation from tips of macroscopic cracks using crack-tip shields for the position of dislocations relative to the tips of cracks and thermomechanical measurements of phase transitions in ZrO_2 for phase transformation fracture toughening.

458. DIFFUSIONAL CREEP OF MULTICOMPONENT SYSTEMS

J. C. M. Li
Dept. of Mechanical Engineering
Phone: (716)-275-4038

$90,994 01-2

Research on stress-motivated diffusion in amorphous and crystalline materials, and elastic plastic deformation in oxide glasses and ceramic, polymeric, and metallic materials. The techniques of "impression" creep, fatigue, load-relaxation and elastic deformation are employed, which utilize very localized loads, and enable determination of localized load-deformation relationships that are representative of bulk behavior. Specific activities include investigations of charged dislocations in KCl, dislocation-crack tip interactions and the density of mobile dislocations.

ROCKWELL INTERNATIONAL SCIENCE CENTER
1049 Camino Dos Rios/Box 1085
Thousand Oaks, CA 91360

459. FABRICATION SCIENCE OF SILICON NITRIDE MATERIALS

F. F. Lange
Phone: (805)-498-4545
P. E. D. Morgan
Phone: (805)-498-4545

$203,681 01-1

Evaluation of the influence of new colloidal precipitation and conventional powder preparation methods for the preparation of Si_3N_4 powder on the microstructure and microchemistry of both green and sintered compacts. Development of a colloidal method for preparing Si_3N_4 synthesis materials by investigating the slip casting of colloidally mixed slips. Study of the Si-S-N chemistry for the synthesis of Si_3N_4 powder. Techniques to obtain a homogeneous distribution of sintering aids and their effect on the resultant microstructure and microchemistry. Development of quantitative methods based on X-ray microanalysis and backscattered electron imaging, for gauging compositional uniformity of powder compacts and sintered materials.

RUTGERS UNIVERSITY
Busch Campus/P. O. Box 909
Piscataway, NJ 08854

460. LOCAL STRUCTURE OF METAL ATOMS IN SILICA AND SILICATES

S. H. Garofalini
Dept. of Ceramics
Phone: (201)-932-2216

$70,092 01-3

Local structure and bulk and surface diffusion of metal ions in vitreous silica and silicated glasses investigated using a combination of extended X-ray absorption fine structure (EXAFS) measurements and computer simulations using molecular dynamics methods. Studies of the effects of local structure, interatomic potential functions, atom size, ion clustering and sample preparation on the mobility of metal species in alkali-zinc-silicates, sol-gel-prepared zinc silicates, and platinum on silica.

RUTGERS UNIVERSITY (continued)

461. HIGH PRESSURE AND SYNCHROTRON RADIATION STUDIES OF SOLID STATE ELECTRONIC INSTABILITIES

J. H. Pifer
Dept. of Physics
Phone: (201)-932-2522
M. C. Croft
Dept. of Physics
Phone: (201)-932-2522

$130,000 02-2

Develop high pressure diamond anvil cell for electron paramagnetic resonance measurements. Study of phase transitions in phosphorus doped silicon, organic charge transfer salts, europium compounds and cesium using this apparatus.

SRI INTERNATIONAL
Menlo Park, CA 94025

462. MINOR ALLOYING ELEMENTS IN THE PITTING BEHAVIOR OF METALS AND ALLOYS

D. D. Macdonald
Chemistry Laboratory
Phone: (415)-859-3195

$114,457 01-3

Experimental and theoretical investigation of pitting in austenitic stainless steels (Fe-Ni-Cr-base composition). Extension of the solute/vacancy interaction model to consider breakdown of passive films and role of minor alloying elements thereon; modelling rate of generation of cation vacancies at the film/solution interface and the interaction between the solutes and vacancies for various solute types (effective valence and concentration). Experimental studies of breakdown characteristics of various alloys in aqueous chloride solutions and possibly other electrolytes. Application of results to alloy design.

SETON HALL UNIVERSITY
South Orange, NJ 07079

463. THE USE OF SURFACE CHARACTERIZED DISPERSED METAL CATALYSTS IN CATALYTIC REACTIONS

R. L. Augustine
Dept. of Chemistry
Phone: (201)-761-9033

$67,522 03-3

The single turnover reaction sequence recently developed for the surface characterization of Pt/CPG catalysts will be expanded as a means of characterizing other catalysts and support combinations. With the availability of these characterized catalysts and the development of a means to prepare catalysts having specific site densities, these catalysts can be used in the study of a variety of catalytic reactions to correlate with those taking place on well characterized surfaces of metallic single crystals and to provide information of value in the preparation of selective and efficient catalysts, for a variety of catalytic processes.

UNIVERSITY OF SOUTHERN CALIFORNIA
Los Angeles, CA 90089-0241

464. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP

T. G. Langdon
Dept. of Materials Science and Mechanical Engineering
Phone: (213)-743-2095

$40,400 (4 Months) 01-2

Measurements of creep and grain boundary sliding in Al and Mg-based alloys stress and temperature dependences; threshold creep stress in precipitation hardened and solid solution strengthened Al-base alloys; boundary migration and sliding in cyclic creep; cavitation in Cu and Cu alloys.

465. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS

F. A. Kröger
Dept. of Materials Science
Phone: (213)-743-6224

$90,000 01-3

Relationship between the composition and microstructure with physical behavior of oxide ceramics, principally Al_2O_3. Relationship of composition, including non-stoichiometry, and microstructure to dopants, conditions of preparation, oxygen fugacity, and temperature, and their effect on physical properties through the defect structure. Experimental studies include electrical conductivity, emf measurements on concentration cells to determine partial ionic and electrical conductivities, electron-spin resonance, optical absorption, and creep.

UNIVERSITY OF SOUTHERN CALIFORNIA (continued)

466. DEPOSITION, MICROSTRUCTURE, AND PROPERTIES OF LASER CVD FILMS

S. D. Allen
Center for Laser Studies
Phone: (213)-743-6705
S. Copley
Dept. of Materials Science
Phone: (213)-743-6223

$130,031 01-5

Experimental and theoretical research on the Laser Chemical Vapor Deposition (LCVD) process to predict deposition rates, microstructures, and resulting film properties. Effects of surface temperature, laser spot size, local vapor composition, total pressure, optical absorption thermal properties, and thermal expansion mismatch are isolated in experiments designed to measure chemical, optical, thermal, and mechanical effects. Calculations and measurements of surface temperature and theoretical analysis of convective transport. Model systems to be investigated include LCVD of SiC on SiC substrates, on SiC substrates coated with Mo, and on Mo and W substrates. Film thickness profiles, microstructures, and film adherence are characterized by a variety of techniques.

SOUTHERN ILLINOIS UNIVERSITY
Carbondale, IL 62901

467. METALLIC GLASSES AS NEW CATALYST SYSTEMS FOR ENERGY CONVERSION

G. V. Smith
Molecular Science Program and Department of Chemistry
Phone: (618)-453-2785,(618)-453-572
W. E. Brower Jr.
Dept. of Mechanical Engineering and Materials
Phone: (618)-536-2396

$40,040 01-1

Selectivity of glassy metallic catalysts related to structure of amorphous metal surfaces and stability of amorphous and nonequilibrium crystalline surface features. Materials studied - Pd-Si, Fe-B, and Zr-Ni alloys prepared by rapid solidification via modified shock tube, hammer and anvil, and single roller techniques. Use of (+)-apopinene as molecular probe for characterizing metallic glasses by correlating with surface features the ratio of isomerization to addition during hydrogenation. Analysis of surface structure with ESCA, ISS, BET surface area, and chemisorption techniques, and of bulk structure with XRD, Mössbauer spectroscopy, TEM, and thermal analyses methods.

SOUTHWEST RESEARCH INSTITUTE
6220 Culebra Road
San Antonio, TX 78284

468. CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION

R. A. Page
Dept. of Materials Science
Phone: (512)-684-5111 X3252
J. Lankford
Dept. of Materials Science
Phone: (512)-684-5111 X2317

$160,084 01-2

Characterization and modeling of cavity nucleation and growth during creep of ceramics using small-angle neutron scattering (SANS), density measurements, transmission electron microscopy (TEM), and Auger electron microscopy. SANS and TEM analysis of pore removal during sintering. Materials under investigation are Al_2O_3, SiC, and Si_3N_4.

STANFORD UNIVERSITY
Stanford, CA 94305

469. INTERNAL-VARIABLE BASED MODELS FOR ELEVATED TEMPERATURE FATIGUE AND DEFORMATION

A. K. Miller
Dept. of Materials Science and Engineering
Phone: (415)-497-3732

$210,000 01-2

Development of a new unified computer model for elevated-temperature fatigue that is based upon explicit representations of the controlling internal physical processes. Related research on the development of a physically-based model of the deformation and ductile failure behavior of metals and alloys including development of improved constitutive equations for multiaxial plasticity and a new model for sheet metal formability under nonproportional strain paths. Research advances earlier modelling work (the development of MATMOD and MATCON constitutive relations) on the plasticity of materials.

STANFORD UNIVERSITY (continued)

470. MECHANISMS OF HIGH TEMPERATURE CRACK GROWTH IN METALS AND ALLOYS

W. D. Nix
Dept. of Materials Science and Engineering
Phone: (415)-497-4259

$85,000	01-2

Study of the processes of creep crack extension in simple metals (Cu and Ni); examination of cavitation damage at crack tip using implanted intergranular cavities and intergranular segregation of Sb in Cu to permit grain boundary fracture in post-creep impact tests; study of the driving forces for crack growth and the temperature dependence of the growth process; examination of the effects of environments on creep crack growth in Ni alloys containing carbon; study of creep crack growth in 304 stainless steel containing different intergranular carbide distributions; theoretical studies of cavitation and crack growth.

471. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

R. H. Bube
Dept. of Materials Science and Engineering
Phone: (415)-497-2534

$197,000	01-3

Interactions occurring at the interface between CdTe with other materials, and the role of interfacial microstructure and microchemistry on the electrical properties of such CdTe containing heterojunctions. Effects of etching and heat treatment on surfaces, Schottky barriers, and heterojunctions formed on CdTe, and the preparation and behavior of polycrystalline films of CdTe. Grain boundary characterization and passivation. Measurements include J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; and diffusion lengths. Scanning transmission electron microscopy and high resolution TEM analysis of heterojunction interfaces; lattice resolution; electron microdiffraction; XPS, Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition, magnetron sputtering, and chemical vapor deposition, and closed-space vapor transport techniques.

472. EVALUATION OF MACHINING DAMAGE IN BRITTLE MATERIALS

B. T. Khuri-Yakub
Dept. of Electrical Engineering
Phone: (415)-497-0718

$94,285	01-5

Investigation of machining damages such as sub-surface slot-like cracks and compressive surface residual stress in brittle materials. Acoustic and laser techniques to measure both the crack sizes and the residual stress. Development of fracture model to predict strength reduction due to machining damage. Slow crack growth effects. Study of Si_3N_4, Si, and SiC.

STANFORD UNIVERSITY (continued)

473. THE USE OF SURFACE ACOUSTIC WAVES TO STUDY SMALL FATIGUE CRACKS

D. V. Nelson
Dept. of Mechanical Engineering
Phone: (415)-497-2123
$130,000 01-5

Study of the growth behavior of fatigue microcracks in 4140 and 300 M steels, as influenced by different microstructures. Monitoring of crack depth and variation in crack closure stress with crack growth using surface acoustic waves as a probe. Comparison of closure stress behavior with that determined by SEM measurements of crack mouth opening displacement vs. applied stress. Measurement by X-ray diffraction of changes in surface residual stresses during fatigue cycling. Correlation of crack growth rate with closure stress behavior, at different stress amplitudes and two mean stress levels. Investigation of the use of an acoustic microscope technique to furnish quantitative information about residual stresses.

STEVENS INSTITUTE OF TECHNOLOGY
Hoboken, NJ 07030

474. STUDIES OF MAGNETISM AND EXCHANGE SCATTERING IN SOLIDS USING SYNCHROTRON RADIATION AND SPIN POLARIZED PHOTOELECTRONS

G. M. Rothberg
Dept. of Materials and Metallurgical Engineering
Phone: (201)-420-5269
$139,000 02-2

A synchrotron light source will be used to produce polarized photoelectrons from transition metal ions. The multiplet splitting serves as the polarizer. Spin polarized EXAFS will be used to study instantaneous short range magnetic order above and below transition temperatures and on surfaces and to study temperature dependence of short range order above transition temperatures.

SYRACUSE UNIVERSITY
Syracuse, NY 13210

475. THE CATALYTIC REACTIVITY TO THIN FILM CRYSTAL SURFACES

R. W. Vook
Dept. of Chemical Engineering and Materials Science
Phone: (315)-423-3466
J. A. Schwarz
Dept. of Chemical Engineering and Materials Science
Phone: (315)-423-4575

$150,000 01-1

Characterization of topography and defect structure on thin film surfaces (Pd, Pt) and of factors that determine their chemical reactivities; measurement of adsorption and desorption (thermal and electron beam induced) kinetics of O_2, CO, and hydrocarbons on these films; work function determination upon gaseous adsorption as a function of surface topography and defect structure; comparison of reactivities of vapor deposited thin film surfaces with similar surfaces that were sputter etched and annealed; chemical reaction investigations at elevated pressures using thin film samples as prototype catalysts that include the effects of catalytic promoters and poisons; techniques used - LEED, AES, EELS, TPD, TEM/TED, RHEED, work function.

UNIVERSITY OF TENNESSEE
Knoxville, TN 37996-1600

476. STATISTICAL MECHANICS OF POLYMER SYSTEMS

J. Kovac
Dept. of Chemistry
Phone: (615)-974-3444

$82,354 03-1

A theoretical investigation into the equilibrium and dynamic behavior of amorphous polymers over a broad range of concentration, molecular weight, and temperature. The investigations involve non-equilibrium thermodynamics, equilibrium and non-equilibrium statistical mechanics, and computer simulation. Specific problems include more realistic models for single chain dynamics, conformation and dynamics of chains in semidilute and bulk systems and equilibrium and dynamic aspects of the glass transition.

UNIVERSITY OF TEXAS
Austin, TX 78712

477. THE NATURE OF PHOTOEMISSION IN DIELECTRIC FLUIDS

J. C. Thompson
Dept. of Physics
Phone: (512)-471-5926
P. R. Antoniewicz
Dept. of Physics
Phone: (512)-471-3766

$115,000 02-2

Photoemission from electrodes into dielectric fluids and time of charge transport studied by pulse injection techniques as function of photon energy, potential, and temperature. Experimental studies: surface roughness, adsorbates, double layer structure, scavengers, solvent structure, laser intensity, and time evolution of charge injection. Density of states calculations and development of models for photoinjection into dielectric media.

UNIVERSITY OF UTAH
Salt Lake City, UT 84112

478. EXPERIMENTAL STUDIES OF THE ELECTRONIC STRUCTURE OF I-II AND I-III INTERMETALLIC COMPOUNDS

I. M. Curelaru
Dept. of Materials Science and Engineering
Phone: (801)-581-3589, 4850, 6863

$80,000 01-1

Systematic investigation of the electron structure of the occupied and empty states for I-II and I-III intermetallic Zintl compounds, with concern for the significance of nonstoichiometry, defect lattice, and degree of localization of conduction orbitals in determining physical behavior. Spectroscopic techniques consist of X-ray photoelectron spectroscopy (XPS), electron energy loss spectroscopy (EELS), core ionization loss spectroscopy (CILS), appearance potential spectroscopy (APS), and extended appearance potential fine structure (EAPFS). Comparison of XPS, EELS, CILS, and APS datta with existing LCAO, cluster model, and self-consistent linear muffin tin LMT band-structure calculations.

UNIVERSITY OF UTAH (continued)

479. FABRICATION, PHASE TRANSFORMATION STUDIES AND CHARACTERIZATION OF SiC-AlN-Al_2OC

A. V. Virkar
Dept. of Materials Science and Engineering
Phone: (801)-581-5396
$99,181 01-1

Preparation of SiC-AlN-Al_2OC powders by a carbothermal reaction of a mixture of SiO_2 and Al_2O_3 in N_2 or argon. Fabrication of SiC-AlN-Al_2OC ceramics by hot pressing, and subjecting such dense, hot pressed ceramics to various annealing treatments. X-ray diffraction and STEM analysis to investigate phase equilibria, precipitate morphology, spinodal decompositions and grain boundaries especially with special regard to the nucleation and growth of possible grain boundary phases. Evaluation of room temperature bend strength and fracture toughness and elevated temperature creep. Emphasis on understanding the inter-relationship of fabrication, microstructure, and mechanical behavior.

480. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V ALLOYS

G. B. Stringfellow
Dept. of Materials Science and Engineering
Phone: (801)-581-8387
$78,083 01-3

Development of an understanding of miscibility gaps in alloys including organometallic vapor phase epitaxy growth of metastable alloys, the effect of short range (100Å to 1000Å) clustering or compositional inhomogeneity in $GaAs_{0.5}Sb_{0.5}$ alloys on hole and electron mobility and photoluminescence half-widths, Raman spectroscopy, and STEM analysis of spinodal compositions and clustering.

VIRGINIA POLYTECHNIC INST. & STATE UNIV.
Blacksburg, VA 24061

481. FRACTURE MECHANISMS IN GLASS-CRYSTAL COMPOSITES

D. P. H. Hasselman
Dept. of Materials Engineering
Phone: (703)-961-5402

$77,000 01-2

Fracture mechanisms in glass-crystal composites with a cordierite glass-ceramic and its original (non-crystallized) glass, glass-alumina composites, and Richterite glass ceramics as the principal materials of study. Flaw introduction by micro-hardness indentation and crack characterization by scanning electron microscopy. Characterization of localized stress distribution near crystalline dispersions, sub-critical and critical crack propagation behavior, associated crack-crystalline interaction, and mechanisms which control the nature (size, geometry) of the fracture-initiating flaw. Biaxial flexure and double torsion of double cantilever beam strength characterizations. Environmental and loading conditions include ambient room air and inert environments, and variable loading rates to establish strain-rate sensitivity.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

482. THE EFFECT OF MICROSTRUCTURE ON THE FATIGUE BEHAVIOR OF FE-C-X ALLOYS

G. J. Shiflet
Materials Science Department
Phone: (804)-924-6340
E. A. Starke Jr.
Materials Science Department
Phone: (804)-924-7097

$60,000 (15 Months) 01-2

Experimental correlation of fatigue behavior of duplex martensitic-ferritic steels; determination of relationship between continuous hard and soft phases (martensite and ferrite) and effects of carbide structure, distribution and morphology as studied by TEM. Control of microstructure by thermomechanical processing of Fe-C-Mn, Fe-C-Mo, Fe-C-V and Fe-C-Mn-V alloys. Correlative studies involving cyclic stress strain response, hardening, softening, microstructure stability under cyclic loading, damage accumulation, crack initiation and propagation in high and low cycle fatigue; micromechanisms, crack closure effects.

UNIVERSITY OF VIRGINIA (continued)

483. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES

R. V. Coleman
Dept. of Physics
Phone: (804)-924-3781

$104,377	02-2

Investigations of the properties of surfaces and interfaces containing molecular adsorbates using elastic electron tunneling spectroscopy (IETS), photoemission (ESCA), and Auger spectrocopies. IETS studies of combinations of oxide substrate and metal overlayer electrodes to establish the nature of the chemical and electronic interactions between molecules and interface: ESCA and Auger studies to augment the IETS work. Studies of UV-induced damage to molecules and photocatalytic effects on semiconductor oxides.

484. MAGNETIC IMPURITIES IN SUPERCONDUCTORS

J. Ruvalds
Dept. of Physics
Phone: (804)-924-3782

$92,423	02-3

Theoretical research on magnetic impurity interactions in superconductors. Investigation of rare earth impurities in various metallic hosts to determine relative importance of exchange interactions and of electronic structural basis for coupling. Studies on influence of impurities, at intermediate concentrations, on the electron spin susceptibility and nuclear spin relaxation rate. Emphasis on new mechanisms for achieving enhancement of superconducting properties in high magnetic fields.

WASHINGTON UNIVERSITY
St. Louis, Missouri 63130

485. NON-EMPIRICAL INTERATOMIC POTENTIALS FOR TRANSITION METALS

A. E. Carlsson
Dept. of Physics
Phone: (314)-889-5739

$55,000 (16 Months)	02-3

Development of existing scheme for calculating interatomic potentials in simplified tight-binding models into a method applicable to transition metals. Consideration of tight-binding models, the tight-binding parameters from a first principles band theory, and effects beyond the extant tight-binding model. Interatomic potentials tested both by experimental data and band theoretic calculations for surfaces and vacancies and subsequently used to calculate the properties of dislocations and grain boundaries.

UNIVERSITY OF WASHINGTON
Seattle, WA 98195

486. NUCLEAR MAGNETIC RESONANCE STUDIES OF LOW MOTION IN FAST ION CONDUCTING SOLIDS

J. L. Bjorkstam
Dept. of Electrical Engineering
Phone: (206)-543-2177
$91,720 01-3

Nuclear magnetic resonance (NMR) studies of fundamental ion transport processes in fast ion conducting crystals and glasses. Measurements of ion dynamics and ion-lattice dynamics in beta aluminas, lithium ion conductors, and borophosphate glasses, and of ion leaching in glasses. The program includes modeling of correlation functions for ion transport in solids and development of improved microprocessor-based NMR instrumentation.

487. X-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls
Dept. of Physics
Phone: (206)-543-2778
$78,000 02-2

Structure and behavior of materials at high pressure by pressure-sensitive phase transformations. The X-ray absorption near-edge structure (XANES) on materials exhibiting structural or thermal disorder-liquid metals and layered compounds.

488. FUNDAMENTAL STUDIES OF ELASTOMERS

B. E. Eichinger
Dept. of Chemistry
Phone: (206)-543-5900
$105,948 03-1

Research to synthesize and characterize elastomers cross-linked by the formation of metal-chelate bonds. Elastomers useful for the determination of the strain dependence of the junction pair correlation function are the primary focus. Theoretical studies to understand network formation processes. Computer simulations of gelation to determine scaling laws for various types of cross-linking systems.

UNIVERSITY OF WEST VIRGINIA
Morgantown, WV 26506

489. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

B. R. Cooper
Dept. of Physics
Phone: (304)-293-3423

$62,351 03-1

Theoretical studies of the crystallographic allotropic transformations of elemental plutonium. Band calculations of the electronic structure, lattice energy, and correlation effects for plutonium and plutonium compounds.

UNIVERSITY OF WISCONSIN
Madison, WI 53706

490. ANALYSIS OF MICROPHASE SEPARATION IN ION CONTAINING POLYMERS

S. L. Cooper
Dept. of Chemical Engineering
Phone: (508)-262-1092

$233,050 (24 Months) 03-1

Investigations of the microstructure of several ionomer systems using techniques which probe different aspects of the structure. Development of a unified model of the morphology which can rationalize the unique physical properties of these materials. Of special interest, the Nafion^{R} ionomers because of their applications in electrochemical processes as selectively permeable membranes. The local arrangement of atoms in the ionic domains studied using Extended X-ray Absorption Fine Structure (EXAFS) analysis and XANES spectroscopy. Information about larger scale structure obtained from X-ray scattering and transmission electron microscopy experiments. To better understand the reason for differences between various ion containing polymers, the effects of several composition and preparation variables explored.

UNIVERSITY OF WISCONSIN (continued)

491. THE STABILITY OF AMORPHOUS METALS ON SEMICONDUCTOR SUBSTRATES

J. D. Wiley
Dept. of Electrical and Computer Engineering
Phone: (608)-263-2354, 1643
J. H. Perepezko
Dept. of Metallurgy and Mineral Engineering
Phone: (608)-263-1678
$84,470 01-1

Experimental investigation of the structure, stability, and atomic transport behavior of high-T_g amorphous-metal films on semiconductor substrates. RF sputtering deposition of thin amorphous films of Ni-Nb, Mo-Si, and W-Si alloys on semiconductor substrates of Si, GaAs, and GaP. Characterization of crystallization kinetics, crystallization mechanisms, and film/substrate interdiffusion at temperatures near the glass-transition temperature by structural, calorimetric, and electrical measurements. Examination of structural relaxation by electrical resistivity measurements during post-deposition annealing. Measurement of diffusion and interdiffusion by a combination of Rutherford backscattering and Auger electron spectroscopy techniques. Assessment of reactions involving crystallization and possible phase separation, involving TEM analysis of in-situ annealing, and supplementary SEM and X-ray diffraction measurements.

492. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

W. M. Yen
Dept. of Physics
Phone: (608)-263-7475
$95,706 02-2

A comprehensive study of relaxation and energy transfer properties of optically-active disordered systems and exploratory investigations of doped ceramics. A capability to measure coherent transient effects developed for use in conjunction with an existing facility for fluorescence line narrowing. Investigation of the temperature dependence of the relaxation effects in disordered materials and testing of disordered materials to determine the microscopic interactions and to extend models. Fundamental study of ion transfer, trapping, and cross relaxation in a prototypical glass system.

UNIVERSITY OF WISCONSIN (continued)

493. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

S. Y. Tong
Dept. of Physics and Surface Studies Laboratory
Phone: (414)-963-4474
$87,000 02-2

Theory of electron energy loss spectroscopy (EELS) and other inelastic scattering at surfaces. Vibrational properties of isolated adatoms and ordered overlayers on metal surfaces, with emphasis on quantitative comparisons with experiment. Role of image potential in large-angle EELS and in LEED studies. Large-angle inelastic scattering from substrate phonons. EELS spectral densities at large wave vector. Surface relaxation, anharmonicity, and surface lattice dynamics. This program coupled to that of D. L. Mills, University of California-Irvine.

XEROX PALO ALTO RESEARCH CENTER
3333 Coyote Hill Road
Palo Alto, CA 94304

494. SEVENTEENTH INTERNATIONAL CONFERENCE ON THE PHYSICS OF SEMICONDUCTORS

R. Z. Bachrach
Phone: (415)-494-4157
$20,000 (24 Months) 02-2

Partial support for the Seventeenth International Conference of Semiconductors, an IUPAP biannual meeting, held August 5-10, 1984 in San Francisco. Some major topics: Electronic States, Impurity States, Excitons, Polaritons, Electron-Hole Liquid and Plasmas, Transport, Recombination, Lattice Dynamics, Low Dimensional Materials, Superlattices and Quantum Wells, Amorphous Semiconductors, and Optical Characteristics. About one thousand to attend.

NATIONAL BUREAU OF STANDARDS
Washington, DC 20234

495. INTERAGENCY PROGRAM FOR SUPPORT OF CRITICAL DATA COMPILATIONS

D. R. Lide - Office of Standard Reference Data
Phone: (301)-921-2467
$200,000

Support for the critical evaluation of data in the physical sciences and for the preparation of compilations of standard reference data is being provided through a collaborative program involving the National Bureau of Standards, National Science Foundation, Office of Naval Research, and the Department of Energy. Thermodynamic and phase equilibria data evaluation and compilation represent the principal thrust of this program.

OAK RIDGE ASSOCIATED UNIVERSITIES
P. O. Box 117
Oak Ridge, TN 37831-0117

A. Wohlpart - Phone (FTS) 626-3421 or (615) 576-3421

496. DOE FACILITY USERS PROGRAM
A. Wohlpart
$140,000 01-1

Collaborative research between university, industry, and national laboratory scientists in materials sciences to foster access to and use of advanced facilities. The SHaRE (Shared Research Equipment Program) facility includes state-of-the-art capabilities in the areas of transmission and analytical electron microscopy, surface analysis, and nuclear microanalysis; approximately 20% of the usage of these facilities is by SHaRE users for basic and applied research on energy-related materials problems, based on research proposals approved by a review committee. The ORSOAR (Oak Ridge Synchrotron Organization for Advanced Research) program involves the National Synchrotron Light Source at the Brookhaven National Laboratory to study the structures of a wide variety of amorphous and crystalline materials including metallic glasses and liquids containing more than one element, heterogeneous catalysts, surface structures, corrosion films, defects and deformed materials, and local atomic arrangements in metal alloys and ceramics; approximately 40% of the beam time will be allocated to users based on a proposal basis.

SECTION C

Small Business Innovation Research

PHASE I SBIR PROJECTS

The goal of the Phase I projects is to determine the technical feasibility of the ideas proposed.

JUPITER INTERNATIONAL
919 East State Street
Ithaca, NY 14850

501. SUPERPLASTIC - FORGING OF STRUCTURAL CERAMICS

Prakash Panda
Staff Scientist
Phone: (607)-273-6054

$50,000 (6 Months) SBIR

To ascertain the feasibility of superplastic forming of engineering ceramic materials, namely, silicon nitride, and glass-ceramic/silicon-carbide-fibre composites. Work will be extended to other candidate materials such as silicon-carbide, zirconia, alumina, spinels and other ceramic-ceramic composites, and CAD/CAM techniques developed and applied to superplastic forming of structural ceramics.

MICROMATERIALS TECHNOLOGY
634 South Main Street
Athens, PA 18810

502. RAPIDLY SOLIDIFIED, SPHERICAL, FINE CERAMIC POWDERS

Richard F. Cheney
Technical Director
Phone: (717)-888-6505

$49,670 (6 Months) SBIR

Determination of the feasibility of making rapidly solidified ceramic powders which are spherical and less than 3 micrometers in average diameter. Rapid solidification technology has been applied to metals with significant improvements in electrical, mechanical, corrosion and wear resistant properties. It is expected that equally significant improvements will be found for ceramics. Properties of the new powders will be evaluated and their densification behavior will be determined using press/sinter and hot-pressing techniques. The properties of selected densified parts will be evaluated.

CERAMATEC INC.
163 West 1700 South
Salt Lake City, UT 84115

503. PROCESSING AND CHARACTERIZATION OF SILICON CARBIDE-ALUMINUM OXYCARBIDE CERAMICS

Raymond A. Cutler
Program Manager
Phone: (801)-486-5071
$49,985 (6 Months) SBIR

To characterize the microstructure and mechanical properties of the sinterable SiC-Al_2OC materials to determine if they are candidates for use in the heat engines, cutting tools, wear parts and other high temperature components. Focus on two methods of synthesizing the desired solid solutions and optimization of processing and composition an important aspect of the study. X-ray diffraction, transmission electron microscopy and energy dispersive spectroscopy used to confirm the existence of a solid solution in the pressureless sintered materials and look at the grain boundary chemistry. Room temperature fracture toughness, hardness, flexural strength and high temperature creep experiments to establish baseline properties and determine the utility of using this new material in high temperature appplications. It is anticipated that SiC-Al_2OC can replace metal bonded carbides (i.e. WC-Co) in some cutting tool applications and thereby reduce the U.S. dependence on cobalt, a strategic metal.

GORHAM INTERNATIONAL
209 Mosher Road
South Windham, ME 04038

504. CONTAINERLESS SINTER/HOT ISOSTATIC PRESSING (HIP) OF A SIALON

Andrew C. Nyce
Materials, Energy and Environmental Division
Phone: (207)-892-2216
$49,993 (6 Months) SBIR

Study is to determine the feasibility of fully densifying a SiAlON via sinter/HIP processing. In this process technology investigation, green preforms are sintered under moderate N_2 pressure to high density and closed porosity in the HIP vessel; following completion of the designated sintering phase of the cycle, the vessel is rapidly pressurized to a suitable HIPing pressure (e.g., 30 KPSI), and the HIP phase of the cycle is then conducted. Sinter/HIP expected to yield technically unique materials with properties and microstructures unlike those produced via other process technologies. The work will aim at fully densifying a 92 wt.% Si_3N_4 + 6 wt.% Y_2O_3 + 2 wt.% Al_2O_3 SiAlON via sinter/HIP. Room temperature modulus of rupture values for sinter/HIPed specimens generated and compared with MOR values for compositionally similar sintered and sintered + containerless HIPed specimens.

KJS ASSOCIATES
1616 Hillrose Place
Fairborn, OH 45342

505. EVALUATION OF METAL-MATRIX COMPOSITES BASED ON FE-ND-3 ALLOYS FOR IMPROVED PERMANENT MAGNETS

Reinhold M. W. Strnat
Research Engineer
Phone: (513)-299-0313, 2717

$49,500 (6 Months) SBIR

Heat-bonded composites of hard magnetic alloy powders in a ductile metal matrix fabricated and characterized for potential high energy permanent magnet applications. The applicability of Sn/Pb-solder bonding to iron-neodymium-boron alloys experimentally explored. Powders of different particle sizes prepared from pre-sintered Fe-Nd-B, compacts of these with solder powder additions made and heat-bonded by immersion in a solder bath. The quality at the bond studied metallographically and by compression tests. Magnetic properties and the composite stability at environmental temperatures up to 150°C. Aging behavior compared with that of sintered Fe-Nd-B and $SmCo_5$, and with polymer and solder-matrix magnets made from Sm-Co and other rare earth-transition metal alloys.

MARKO MATERIALS INC.
144 Rangeway Road
North Billerica, MA 01862

506. RAPIDLY SOLIDIFIED MAGNETIC ALLOYS FOR HIGH FREQUENCY, HIGH POWER APPLICATIONS

Ranjan Ray
President
Phone: (617)-663-2210

$50,000 (6 Months) SBIR

Metallic glasses fill a magnetic materials gap between nickel-iron soft magnetic alloys (the permalloys) and soft ferrites; show outstanding promise as a low loss, high-magnetic-induction core materials for the growing high-frequency, high-power applications markets. While hysteretic losses are known to originate from magnetoelastic interactions, the exact mode of coupling is not known. A model of the coupling is proposed which, if proven to be correct, should aid in designing transformer cores of lower loss. A series of measurements will be carried out to determine whether to avoid these losses through use of a non-magnetostrictive, cobalt-base glass or through more careful heat treatment of the higher induction but magnetostrictive iron-base amorphous alloys.

TECHNICAL RESEARCH ASSOCIATES INC.
410 Chipeta Way, Suite 222
Salt Lake City, UT 84108

507. OXIDE DISPERSION STRENGTHENED (ODS) TUNGSTEN CARBIDE-COBALT

Guy B. Alexander
Senior Vice President
Phone: (801)-582-8080

$49,718 (6 Months) SBIR

Cobalt is a strategically important element, and minimizing its use is a problem of national significance. Cobalt is used in cemented carbides, particularly tungsten carbide-cobalt, which are in turn used for metal cutting, mining tools, wire drawing dies and the like. In this program, a novel way to improve the properties of WC-Co alloys, and thus improve the use life of such alloys in cutting tools, mining tools, etc. will be investigated. WC-Co alloys of higher hardness at a fixed rupture strength and/or higher strength at fixed hardness and the use life of such new materials will be grossly improved. These improvements will occur because the tungsten carbide will be slightly finer grained than in conventional alloys, carbon content will be very tightly controlled, and the cobalt will be oxide dispersion strengthened.

AMERICAN RESEARCH CORPORATION OF VIRGINIA
642 First St., P.O. Box 3406
Radford, VA 24143-3406

508. EDDY CURRENT NONDESTRUCTIVE EVALUATION OF LASER GLAZED METALLIC SURFACES

R. J. Churchill
President
Phone: (703)-639-9542

$49,873 (6 Months) SBIR

An investigation using eddy current nondestructive evaluation (NDE) techniques to achieve control of surface layers and to identify defects in surface regions modified in terms of microstructure and/or composition with laser heating. The target: establish a suitable laser glazing model, determine the applicability of eddy current NDE techniques, measure properties of laser glazed layers in known alloys and in cast iron and high speed steels of interest in energy-related industries, and optimize the system parameters. This will facilitate the controlled fabrication of quality amorphous films that exhibit superior properties with respect to corrosion and strength.

PHASE II SBIR PROJECTS

The Phase II projects are a continuation of the successful Phase I projects. The goal of the Phase II projects is to determine commercial feasibility.

CERAMIC FINISHING COMPANY
P. O. Box 498
State College, PA 16804

511. FRACTURE MECHANICS INVESTIGATION OF GRINDING OF CERAMICS

Henry P. Kirchner
President
Phone: (814)-238-4270

$107,988 SBIR

Application of contact fracture mechanics to investigate mechanisms of material removal and damage penetration during abrasive machining of ceramics. Phase I research investigated the mechanisms of material removal including crushing by mixed mode fracture ahead of the diamond point and chipping at lateral cracks propagating in response to residual stresses induced by elastic relaxation against the irreversibly deformed zone on unloading. The objectives: determine the relative importance of crushing ahead of the diamond point and chipping alongside the track as a result of lateral cracking, for various material properties and grinding conditions, investigate the role of crushing in reducing the residual stresses that are responsible for lateral cracking, develop mathematical models by adapting available models for static indentations. The experimental results will be compared with results predicted by these models.

CERES CORPORATION INC.
202 Boston Road
North Billerica, MA 01862

512. HORIZONTAL GROWTH OF SILICON SHEET CRYSTALS VIA EDGE-SUPPORTED PULLING (ESP) FROM MELT CONTAINED IN A COLD CRUCIBLE

Joseph F. Wenckus
President
Phone: (617)-899-5522

$142,510 SBIR

Explore the feasibility of growing silicon sheet crystals horizontally using the edge-supported pulling (ESP) process from silicon melts contained in an RF heated crucible. The vertical edge-supported pulling (ESP) process provides exceptionally stable sheet growth conditions, but sheet growth rates achieved to date are severely restricted by the rate of heat dissipation from the narrow sheet/melt interface. This program endeavors to integrate the unique operational features of the cold crucible with the equally unique attributes of the ESP process to demonstrate the feasibility of the horizontal edge-supported pulling (HESP) method for the production of silicon crystals.

ELECTROCHEMICAL TECHNOLOGY CORPORATION
3935 Leary Way, N.W.
Seattle, WA 98107

513. MATHEMATICAL MODELING OF ELECTROCHEMISTRY OF STRESS CORROSION CRACKING

T. R. Beck
Phone: (206)-632-5965
$167,586 SBIR

Mathematical modeling of the electrochemical transport and kinetic processes that occur in tunnel corrosion of aluminum; correlative experiments on salt film properties using the shielded electrode technique; relation of the above to stress corrosion cracking.

SUPERCON INC.
9 Eric Drive
Natick, MA 01760

514. INVESTIGATION TO DETERMINE THE COMMERCIAL FEASIBILITY OF IN SITU CU-NB COMPOSITES FOR HIGH STRENGTH, HIGH CONDUCTIVITY APPLICATION

J. Wong
Phone: (617)-655-0500
$233,333 SBIR

Development of a procedure for determining the commercial feasibility of fabricating 'in situ' Cu-Nb multifilamentary composites for high stress, high conductivity applications. Maintenance of a low volume fraction of Nb to retain desirable electrical and thermal properties of Cu. Evaluation of composite formability, tensile and fatigue strengths, and electrical conductivity.

UNIVERSAL ENERGY SYSTEMS INC.
4401 Dayton-Xenia Road
Dayton, OH 45432

515. FABRICATION OF AMORPHOUS METALLIC FILMS AND COATINGS FOR INDUSTRIAL APPLICATION USING HIGH ENERGY ION BEAM MIXING

Peter P. Pronko
Chief Scientist
Phone: (513)-426-6900
$249,990 SBIR

Fabrication of amorphous Ni- and Cu-base metallic films and coatings using deeply penetrating high energy ion beam mixing. Use of the so-called structural difference rule for amorphous alloy formation by ion mixing. Evaluation of modified surfaces in erosive and corrosive pitting conditions, e.g. involving exposure to electro-hydrodynamic and corrosive fluid dynamic environments and comparison with crystalline metal behavior.

SECTION D

Collaborative Research Centers

Basic materials research which is long range, generic in nature is supported by the Office of Basic Energy Sciences/Division of Materials Sciences to provide an underpinning for the development of energy technologies. In the pursuit of this research goal, facilities or centers have been and are being developed which are unique and/or expensive and costly to reproduce. Scientists from other laboratories outside of the host laboratory are encouraged to make use of these unique facilities. In this section, a description is included for most of the important centers together with a statement of the method of gaining access to them. Collaborations carried out by outside users have to be in the furtherance of DOE objectives. Any activity which can be carried out through commercially available laboratories is not appropriate for these DOE centers. Proprietary research cannot be conducted unless there is full cost recovery. Each center has a slightly different mode of operation tailored to its best use. For more information, please contact the laboratory personnel listed.

D-1

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, New York 11973

The National Synchrotron Light Source (NSLS) facility consists of a 750 MeV (9 electron bunch) storage ring for VUV and IR research and a 2.5 GeV (30 electron bunch) storage ring for X-ray research. Attractive features of the synchrotron radiation include high brightness and intensity, its broad and continuous spectral range, high polarization and pulsed time structure (subnanosecond pulses). With each of the 28 X-ray and 16 VUV beam ports being further split into from 2 to 4 beam lines, it will be possible to have as many as 100 experiments running simultaneously at the NSLS. A 6 pole superconducting wiggler magnet and a 38 period permanent magnet undulator have been constructed, and several wiggler and undulator magnets are presently being designed which will significantly increase the photon intensity and brightness.

The NSLS is a facility where a wide range of research techniques will be utilized by solid state physicists, metallurgists, biologists, chemists, and engineers for basic and applied studies. Among the techniques are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

USER MODE

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines are being designed and instrumented by "Participating Research Teams" (PRTs). The PRTs are given priority for up to 75% of their beam line(s) operational time for a three-year term.

General Users will be able to perform experiments on an NSLS facility beam line or on a PRT beam line which will be available for use by non-PRT members for at least 25% of its total operational time. In the latter case, PRTs will provide liaison and utilization support to General Users. After an initial commissioning period, NSLS and PRT beam lines will become available for use by General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee will be charged for the amount of beam time utilized. The DOE has granted the NSLS a Class Waiver, under the terms of which Proprietary Users of the NSLS will have the option to retain title to inventions that result from research performed at the Light Source.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky
NSLS - Bldg. 510E
Brookhaven National Laboratory
Upton, New York 11973

(516) 282-4974
(FTS) 666-4974

D-2

NATIONAL SYNCHROTRON LIGHT SOURCE

TECHNICAL DATA

Facilities	Key Features	Operating Characteristics
VUV electron storage ring	high brightness, continuous wavelengh range (λ > 5 Å) 16 beam ports.	0.75 GeV electron energy
X-ray electron storage ring	high brightness, continuous wavelength range (λ > .5 Å) 28 beam ports	2.5 GeV electron energy
Instruments		
Monochromators:		
plane grating	12 Å < λ < 1500 Å; high resolution	
zone plate	8 Å < λ < 100 Å; moderate resolution	
toroidal grating	10 Å < λ < 2500 Å; high intensity, moderate and high resolution	
extended range grasshopper	10 Å < λ < 2000 Å; high resolution	
Wadsworth	300 Å < λ < 3000 Å; high intensity, moderate resolution	
Seya & Czerny Turner	1200 Å < λ < 12000 Å; high intensity, moderate resolution	
two crystal	.04 Å < λ < 2500 Å; high resolution, fixed exit beam	
two crystal/two grating	2.5 Å < λ < 2500 Å; high resolution, fixed exit beam	
Six circle spectrometer/ diffractometers	high positional and rotational accuracy	
Experimental stations	photoemission, magnetic circular dichroism, fluorescence, gas phase spectroscopy, microscopy, lithography, holography, EXAFS, inelastic scattering, crystallography, radiometry, topography, small angle scattering	
Superconducting wiggler	λ > .1 Å; high intensity	
Permanent magnet undulator	30 Å < λ < 5000 Å; high intensity and brightness	

D-3

HIGH FLUX BEAM REACTOR

Brookhaven National Laboratory
Upton, New York 11973

The Brookhaven High Flux Beam Reactor (HFBR) operates at a power of 60 megawatts and provides an intense source of thermal neutrons (total thermal flux = 1.0×10^{15} neutrons/cm^2-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($\lambda > 4$ Å). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure are also available. The emphasis of the research efforts at the HFBR has been on the study of fundamental problems in the fields of solid state and nuclear physics and in structural chemistry and biology.

USER MODE

The HFBR serves the U.S. scientific community and there exists a strong collaboration between the Brookhaven staff and users from universities, industry, and other national laboratories. In 1982 more than 160 persons from outside institutions participated in experiments at Brookhaven. Experiments are scheduled at the HFBR following review of research proposals. Please contact R. Klaffky for more information and for a copy of the HFBR Handbook which contains considerable detail on the available equipment and on operating procedures.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the National Synchrotron Light Source or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky
NSLS - Bldg. 510E
Brookhaven National Laboratory
Upton, New York 11973

(516) 282-4974
FTS 666-4974

HIGH FLUX BEAM REACTOR

TECHNICAL DATA

Instruments	Purpose and Description
Solid State Physics	
4 Triple-axis Spectrometers	Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: $2.5 \text{ meV} < E_o < 200 \text{ meV}$ Q range: $0.03 < Q < 10\text{Å}^{-1}$
Biology	
Small Angle Neutron Scattering	Studies of large molecules. Located on cold source with 20 x 20 cm^2 position-sensitive area detector. Sample detector distance $L < 2$ meter Incident wavelength $4\text{ Å} < \lambda_o < 10\text{ Å}$
Diffractometer	Protein crystallography 20 x 20 cm^2 area detector $\lambda_o = 1.57\text{ Å}$
Chemistry	
2 Diffractometers	Single-crystal elastic scattering 4-circle goniometer $1.69\text{ Å} < \lambda_o < 0.65\text{ Å}$
1 Triple-axis Spectrometer	Inelastic scattering Diffuse scattering Powder diffractometry
Nuclear Physics	
3 Spectrometers	Neutron capture studies Energy range: $0.025\text{eV} < E_o < 25\text{keV}$
TRISTAN II (Isotope Separator)	Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission
Irradiation Facilities	
7 Vertical Thimbles	Neutron activation; production of isotopes; thermal flux: $8.3\text{x}10^{14}$ neutrons/cm^2 sec; fast (>0.5 MeV) flux: $3\text{x}10^{14}$ neutrons/cm^2 sec.

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NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Solid State and Chemistry Divisions
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, fluxoid lattices in superconductors, liquid structures, and crystal structures. The HFIR is a 100-MW, light-water moderated reactor with an unsurpassed record of operating time (better than 90%). The central flux is 5×10^{15} neutrons/cm^2 sec, and the flux at the inner end of the beam tubes is slightly greater than 10^{15} neutrons/cm^2 sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Three of these are unique within this country: the double-crystal small-angle diffractometer, the correlation chopper, and the wide-angle time-slicing diffractometer.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an internal review committee. It is expected that all accepted experiments will be scheduled within six months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be borne by the user. Financial assistance is available for the travel and living expenses of users from U.S. universities. Inexperienced users will normally collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full cost recovery, including a charge for beam time. A brochure describing the facilities and a booklet giving user procedures are available on request.

PERSON TO CONTACT FOR INFORMATION

H. A. Mook
Solid State Division
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

(615) 574-5242
FTS 624-5242

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NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

TECHNICAL DATA

Beam No.	Instrument	Operating Characteristics
HB-1	Triple-axis polarized-beam	Beam size - 2.5 by 3 cm max. Flux - 2.6 x 10^6 neut/cm^2 sec at sample (polarized) Vertical magnetic fields to 5 T Horizontal fields to 2 T Variable E_o
HB-1A	Triple-axis, fixed E_o	E_o = 14.7 meV, 2.353 Å Beam size - 5 by 3.7 cm max. Flux - 9 x 10^6 neut/cm^2 sec at sample with 40' collimation
HB-2A	Liquid diffractometer with linear position sensitive detector	Beam size - 1 by 3.4 cm max. λ = 0.89 Å Flux - 6.8 x 10^5 neut/cm^2 sec at sample with 20' collimation
HB-2, HB-3	Triple-axis, variable E_o	Beam size - 5 by 3.7 cm max. Flux - 10^7 neut/cm^2 sec at sample with 40' collimation
HB-3A	Double-crystal small-angle diffractometer	Beam size - 4 x 2 cm max. Flux - 10^4 neut/cm^2 sec λ = 2.6 Å Resolution - 4 x 10^{-5} $Å^{-1}$
HB-4A	Four-circle diffractometer	Beam size - 5 x 5 mm Flux - 2 x 10^6 neut/cm^2 sec with 9' collimation λ = 1.015 Å
	Wide-angle time-slicing diffractometer	Beam size - 2 x 3.7 cm max. Flux - 2 x 10^6 neut/cm^2 sec with 9' collimation λ = 1.015 Å Curved linear position sensitive detector covering 130°
HB-4	Correlation chopper	Beam size - 5 x 3.7 cm Flight path - 1.5 m 70 detectors covering 130° Variable E_o Variable pulse width

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INTENSE PULSED NEUTRON SOURCE

Argonne National Laboratory
Argonne, Illinois 60439

IPNS is an intermediate level pulsed spallation source dedicated to research on condensed matter. The peak thermal flux is about 3×10^{14} n/cm^2 sec. The source has some unique characteristics that promise to open up new scientific opportunites:

- high fluxes of epithermal neutrons (0.1-10 eV)
- pulsed nature, suitable for real-time studies and measurements under extreme environment

Two principal types of scientific activity are underway at IPNS: neutron diffraction, concerned with the structural arrangement of atoms (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties and inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momemtum with the system under study and thus probes the dynamics of the system at a microscopic level. At the same time, it is expected that the facilities will be used for fundamental physics measurements as well as for technological applications such as stress distribution in materials and characterization of zeolites, ceramics and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS, Building 360, Argonne National Laboratory.

PERSONS TO CONTACT FOR INFORMATION

G. H. Lander, Program Director	(312) 972-5518 FTS 972-5518
B. S. Brown, Operations Manager	(312) 972-4999 FTS 972-4999
T. G. Worlton, Scientific Secretary	(312) 972-8755 FTS 972-8755

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

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IPNS-I EXPERIMENTAL FACILITIES

NEUTRON SCATTERING

Facility (Instrument Scientist)	Assignment	Range †Wave-vector	Range Energy	Resolution Wave-vector	Resolution Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-50 Å^{-1}	*	0.35%	*
General Purpose Powder Diffractometer (J. Faber, Jr.)	F2	0.5-100 Å^{-1}	*	0.25%	*
Single Crystal Diffractometer (A. J. Schultz)	H1	2-20 Å^{-1}	*	2%	*
Low-Resolution Medium-Energy Chopper Spectrometer (C.-K. Loong)	F4	0.1-30 Å^{-1}	0-0.6 eV	0.02 K_o	0.05 E_o
High-Resolution Medium-Energy Chopper Spectrometer (D. L. Price)	H3	0.3-9 Å^{-1}	0-0.4 eV	0.01 K_o	0.02 E_o
Small-Angle Scattering Diffractometer (J. E. Epperson)	C1	0.008-0.3 Å^{-1}	*	0.004 Å^{-1}	*
Crystal Analyzer Spectrometer (T. O. Brun)	F1	3-16 Å^{-1}	0.02-0.5 eV	3%	2%

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* No energy analysis

† Wave-vector, $K = 4\pi \sin \theta/\lambda$

NEUTRON BEAMS FOR SPECIAL EXPERIMENTS

Beam Tube	Current Use	Flight Path Length (m)
F3	eV Spectrometer	10
C2	Polarized Neutron Exp.	10
C3	Solid He^3 Project	10
F6	Irradiations	6-20
H2	Irradiations	6-20
V1	Ultra-Cold Neutron Exp.	4

SNR/PSR SPALLATION NEUTRON SOURCE

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The SNR/PSR (Spallation Neutron Research/Proton Storage Ring) facility is a pulsed spallation neutron source driven by the 800-MeV Los Alamos Meson Physics (LAMPF) linear accelerator. Neutron scattering research is currently carried out at the SNR using the advantages of time-of-flight methods. The facility supports a national neutron scattering user program. Available instruments in the user program are: a) a general purpose powder diffractometer; b) a single crystal diffractometer based on the Laue-TOF technique; and c) a filter difference spectrometer for chemical and optic mode spectroscopy. A considerable effort is directed toward pulsed source instrument development including, currently, a constant Q spectrometer, a chopper spectrometer, an electron volt spectrometer, and a liquid and amorphous diffractometer. A proton storage ring (PSR) is under construction and by 1985 the SNR/PSR will provide at 12 neutron bursts per second the world's highest peak thermal flux for neutron scattering research. In addition, it will also be a source of epithermal neutrons many orders of magnitude larger than reactors for neutron scattering research in solid state physics, chemistry, biology, polymers, and materials science.

USER MODE

Two thirds of the neutron scattering beam time on user instruments at the SNR/PSR is allocated by a nationally appointed Program Advisory Committee. Application for instrument time can be made by submitting a completed proposal form for consideration by the PAC. The PAC evaluates proposals on the basis of scientific excellence and optimal use of SNR/PSR capabilities. One third of the neutron scattering beam time is reserved for Laboratory discretionary research, research pertinent to DOE applied program goals, and instrument development. The SNR/PSR instrumentation is available without charge for nonproprietary research. The facility is open to all U.S. citizens and permanent resident aliens, and to visits of less than seven working days for citizens of non-sensitive countries. DOE approval is required for any other foreign national visits.

PERSON TO CONTACT FOR INFORMATION

R. N. Silver
MS H805, Group P-8
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-6069, or
(FTS) 843-6069

SNR/PSR

TECHNICAL DATA

	1984	1985
Proton Source	LAMPF	LAMPF + PSR
Proton Source Current	1000μA	1000μA
Proton Source Energy	800MeV	800MeV
SNR Proton Current	5μA	100μA
Proton Pulse Width	6μs	0.27μs
Repetition Rate	120Hz	12Hz
Epithermal Neutron Current (n/eV.Sr.S)	$1.6X10^{11}/E$	$3.2X10^{12}/E$
Peak Thermal Flux ($n/cm^2.S$)	$5x10^{13}$	$2x10^{16}$

User Instrument	
General Purpose Powder Diffractometer	Liquids and amorphous metals, powder diffraction wave vector 0.3-50A^{-1} resolution 0.45% powder 2% liquids
Single Crystal Diffractometer	Laue time-of-flight spectrometer wave vector 1-15A^{-1} resolution 2% typical
Filter Difference Spectrometer	Inelastic neutron scattering, vibrational spectroscopy energy trans. 35-600 MeV resolution 5-7%

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NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The National Center for Small-Angle Scattering Research is supported by the National Science Foundation and the Department of Energy under an interagency agreement. The two main instruments available to users are the NSF-constructed 30-m small-angle neutron scattering facility (SANS) and the DOE-constructed 10-m small-angle x-ray scattering camera (SAXS). These instruments are intended to provide state-of-the-art capability for investigating structures of condensed matter on a global scale, e.g., from a few tens to several hundreds of angstroms. They are intended to serve the needs of scientists in the areas of biology, polymer science, chemistry, metallurgy and materials science, and solid state physics.

USER MODE

Beam time on these instruments is assigned, in general, on the basis of proposals submitted in advance. These are then reviewed by a panel of experts external to the Laboratory and are rated on the basis of scientific merit. When a favorable review has been received, a staff member of the NCSASR and the user agree, usually by telephone, on a time and duration for the experiment. Ordinary charges are borne by the Center, but extensive use of support facilities (shops, computing, etc.) must be paid by the user. Users may work in collaboration with one or more staff members if they wish, but such collaboration is not required. Proprietary experiments can be carried out after contractual agreement has been reached.

PERSONS TO CONTACT FOR INFORMATION

W. C. Koehler, Director NCSASR	(615) 574-5232	FTS:	624-5232
G. D. Wignall, SANS-NCSASR	(615) 574-5237	FTS:	624-5237
J. S. Lin, SAXS-NCSASR	(615) 574-4534	FTS:	624-4534
G. J. Bunick, SANS-NCSASR	(615) 576-2685	FTS:	626-2685
M. Gillespie, Secretary NCSASR	(615) 574-5231	FTS:	624-5231

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

TECHNICAL DATA

30-m SANS Instrument Specifications

Monochromator: six pairs of pyrolytic graphite crystals

Incident wavelength: 4.75 Å or 2.38 Å

Wavelength resolution: $\Delta\lambda/\lambda = 6\%$

Source-to-sample distance: 10 m

Beam size at specimen: 0.5–3.0 cm diam

Sample-to-detector distance: 1.5–18.5 m

K range: $5 \times 10^{-3} \leq K \leq 0.6$ Å^{-1}

Detector: 64 by 64 cm^2

Flux at specimen: 10^4–10^6 neutrons/cm^2 sec depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite

Incident wavelengths: 1.542 Å (CuK_α) or 0.707 Å (MoK_α)

Source-to-sample distances: 0.5, 1.0, 1.5. . . ., 5.0 m

Beam size at specimen: 0.1 by 0.1 cm (fixed)

Sample-to-detector distances: 1, 1.5, 2.0, ..., 5 m

K range covered: $3 \times 10^{-3} \leq K \leq 0.3$ Å^{-1} (CuK_α)
$6 \times 10^{-3} \leq K \leq 0.6$ Å^{-1} (MoK_α)

Maximum flux at specimen: 10^6 photons per second on sample-irradiated area 0.1 by 0.1 cm

Detector: 20- by 20-cm^2 (electronic resolution 0.1 by 0.1 cm^2)

Special features: deformation device for dynamic scattering experiments (time slicing in periods as short as 100 μs for oscillatory experiments or 10 s for transient relaxation experiments) and interactive graphics for data analysis

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STANFORD SYNCHROTRON RADIATION LABORATORY

Stanford University
Stanford, California 94305

SSRL is a national facility for the utilization of synchrotron radiation. The radiation comes from the 4 GeV storage ring, SPEAR. SPEAR is dedicated to the production of synchrotron radiation half of its operating time. During this time, high currents (up to 100 mA) of electrons are stored at high energy (3-3.5 GeV). The other half of the time, the ring operates for both colliding beam physics and synchrotron radiation under conditions established by the high energy physics program.

Specific research performed at SSRL is extremely varied and includes, in the vacuum ultraviolet area: ionization properties of small molecules, structural and electronic properties of microstructures, properties of ultra-thin layers and small clusters, kinetic process in laser materials, lithography and microscopy, and static properties and dynamic processes of chemisorbed gases. Presently research in the chemical and biological sciences includes: the structure and function of homo- and heterogeneous catalysts, the structure of metal, metal oxide and semiconductor surfaces and their interactions with small molecules, chemical reactivities in the gas phase, the structure of general chemical compounds through EXAFS, multiple wavelength imaging, protein structures and functions through diffraction studies in the crystalline state, protein structures through EXAFS studies, dynamics and fluctuations in biological systems, the nature of membrane structures and membrane protein interactions, the structure and function of metal site in metalloproteins and metalloenzymes.

X-ray physics and materials sciences are represented by research in the following areas: structure of amorphous materials, coordination of impurities and alloying species, structures of and phase transitions in surfaces and thin surface layers, kinetics of structural changes in materials, phase transitions at high pressure, structure of crystalline materials, electronic structure of materials through edge absorption studies, fundamental X-ray scattering and absorption physics, and atomic physics.

Presently SSRL has 18 experimental stations on 6 beam lines covering the spectrum from 6-45,000 eV. A wide variety of experimental equipment is available for the user and there are no charges either for use of the beam or for the facility-owned support equipment.

USER MODE

SSRL is a user-oriented Facility which welcomes proposals for experiments from all qualified scientists. Access is gained through proposal submittal and peer review. In the course of a year approximately 60% of all active proposals receive beam time.

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell
SSRL, Bin 69 P. O. Box 4349
STANFORD, CA 94305

(415) 854-3300 ext. 3191
(FTS) 461-9300 ext. 3191

CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

	Horizontal Angular Acceptance (Mrad)	Energy Range (eV)	Resolution	Approximate Spot Size Hgt x Wdth (mm)	Remarks
Beam Line I					
1-1 (4°)	2.0	32-1000	$\Delta\lambda \approx .1-.2$Å	2.0 x 1.0	Double Focus
1-2 (8°)	4.0	4-40	$\Delta\lambda \approx .2-6$Å	1.0 x 3.0	Highly Polarized Double Focus
1-4 (Curved Crystal)	2.2	6000-9500	~ 60 eV	0.25 x 0.5	Double Focus Scattering
1-5 (EXAFS I)	1.0	3800-29300	$\Delta\lambda E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line II					
II-2	4.8	2800-8900	$\Delta E/E \sim 5 \times 10^{-4}$	2.0 x 4.0	Rapidly Tunable
II-3	1.0	2800-30000	$\Delta E/E \sim 5 \times 10^{-4}$	2.0 x 20.0	Rapidly Tunable
II-4	1.0	3200-30000	White Radiation	4.0 x 15.0	
Beam Line III					
III-1 (4°)	2.0	15-1200	$\Delta\lambda \approx .05-2$Å	1.0 x 1.0	Double Focus
III-3 (2°)	8-10	800-4000	0.35-7 eV	2.0 x 4.0	Ultra High Vacuum
III-4 (3°)	2.0	2-3000	White or $\Delta\lambda/\lambda \approx .01$	2 x 8	Differentially Pumped
Beam Line IV (Wiggler)					
IV-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	4.6	2800-10200	$\Delta E/E \sim 5 \times 10^{-4}$	2.0 x 6.0	
IV-3 & IV-1	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line VI (Wiggler)					
VI-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	3.0	2800-21000	$\Delta E/E \sim 5 \times 10^{-4}$	2.0 x 6.0	
Beam Line VII (Wiggler)					
VII-1 (Rotation Camera)	1.0	4500-8500	$\Delta E/E \sim 8 \times 10^{-4}$	0.6 x 3.0	Double Focus
VII-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	4.6	2800-10200	$\Delta E/ \sim 5 \times 10^{-4}$	2.0 x 6.0	
VII-3	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line 0-0 (Lifetimes Port)	1.8	1-6	Bandpass 10Å	4.0 x .4	Pulsed Visible Light

June 18, 1984

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory Electron Microscopy Center for Materials Research provides unique facilities which combine the techniques of high-voltage electron microscopy, ion-beam modification, and ion-beam analysis, along with analytical electron microscopy.

The cornerstone of the Center is a High Voltage Electron Microscope (an improved Kratos/AEI EM7) with a maximum voltage of 1.2 MV and a demonstrated lattice resolution of 3.5 Å. This HVEM is interfaced to two accelerators, a National Electrostatics 2MV Tandem Ion Accelerator and a Texas Nuclear 300 kV ion accelerator, which can produce ion beams from 10 keV to 8 MeV of most stable elements in the periodic table. These instruments together comprise the unique High-Voltage Electron Microscope-Tandem Accelerator Facility. The available ion beams can be transported into the HVEM to permit direct observation of the effects of ions and electrons on materials. In addition to the ion-beam interface, the HVEM has a number of specialized features (see opposite page), which allow for a wide range of in situ experiments on materials under a variety of conditions.

In addition to the HVEM-Tandem Facility, the Center's facilities include a JEOL 100 CX transmission and scanning transmission electron microscope (TEM/STEM), equipped with an x-ray energy dispersive spectrometer (XEDS), and a Philips EM 400 TEM equipped with XEDS and an electron energy loss spectrometer (EELS). Procurement of an advanced Analytical Electron Microscope (AEM) is underway. This state-of-the-art, ultra-high vacuum AEM will operate up to 300 keV and have the highest available microanalytical resolution. As such, it will have substantially increased analytical capabilities for materials research over present-day instruments.

USER MODE

The Center is operated as a national resource for materials research. Qualified scientists wishing to conduct experiments using the unique facilities of the Center should submit a proposal to the person named below. Experiments are approved by a Steering Committee following peer evaluation of the proposals. There are no use charges for basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

PERSON TO CONTACT FOR INFORMATION

A. Taylor (312) 972-5109
Electron Microscopy Center for Materials Research FTS 972-5109
Materials Science and Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

TECHNICAL DATA

Electron Microscopes	**Key Features**
High-Voltage Electron Microscope Kratos/AEI EM7 (1.2 MeV)	Resolution 3.5 Å lattice Magnification 63-1,000,000X Continuous voltage selection (100-1200 kV) Curent density 15 A/cm^2 High-vacuum specimen chamber Negative-ion trap Electron and ion dosimetry systems Video recording system Ion-beam interface Specimen stages 10 K - 1300 K Straining and environmental stages
Transmission Electron Microscope Philips EM 400 (120 keV)	Resolution 2.0 Å lattice Equipped with EELS, XEDS Specimen stages 78 K - 900 K
Transmission Electron Microscope JEOL 100 CX (120 keV)	Resolution 2.0 Å lattice Equipped with STEM, XEDS Specimen stages 78 K - 900 K
Analytical Electron Microscope Being acquired (300 keV)	State-of-the-art resolution Ultra-high vacuum Equipped with EELS, XEDS, etc.
Accelerators	
NEC Model 2 UDHS	Terminal voltage 2 MV Energy stability ± 250 eV Current density: H^+, 10 $\mu A/cm^2$ (typical) Ni^+, 3 $\mu A/cm^2$
Texas Nuclear 300-kV	Terminal voltage 300 kV Energy stability ± 300 eV Current density: He^+, 200 $\mu A/cm^2$ (typical) Ni^+, 2 $\mu A/cm^2$

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SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The microanalysis facilities for use in materials science have been made available for collaborative research by members of universities or industry with ORNL staff members. The facilities include state-of-the-art analytical transmission electron microscopy, high voltage electron microscopy, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include high resolution, high voltage in situ studies, and analytical [energy dispersive x-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS), and convergent beam electron diffraction (CBED)]. Surface analysis facilities include four Auger electron spectroscopy (AES) systems; ion backscattering and nuclear reaction techniques using the 0.4 and 5.0 MV Van de Graaff accelerators in the Metals and Ceramics Division.

USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, P. S. Sklad, J. J. Hren, R. F. Davis, and R. E. Wiesehuegel. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and must identify one ORNL staff member who will share responsibility for the project.

The SHaRE program provides technical help and limited travel expenses for academic participants through the Oak Ridge Associated Universities (ORAU).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik Metals and Ceramics Division Oak Ridge National Laboratory Oak Ridge, Tennessee 37830	(615) 574-5066 FTS 624-5066
A. Wohlpart Oak Ridge Associated Universities P.O. Box 117 Oak Ridge, Tennessee 37830	(615) 576-3422 FTS 626-3422

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SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Instruments and Facilities	Key Features	Operating Characteristics
Hitachi HU-1000 High Voltage Electron Microscope	Heating stages; in situ deformation stages; low light level videorecording system; environmental cell — 0–1 atm	0.3–1.0 MeV; electron irradiation studies; ten 4-h shifts/week; available evenings, weekends to qualified users
Philips EM400T/FEG Analytical Electron Microscope	TEM resolution <0.16 nm; STEM resolution <1.0 nm; EDS, EELS, CBEB	120 kV; ten 4-h shifts/week; available evenings, weekends, to qualified users; structural and elemental microanalysis; minimum probe diameter <1 nm
JEOL 120CX Analytical Electron Microscope	TEM resolution ~0.34 nm; STEM resolution ~3 nm; EDS, EELS, CBED	120 kV; ten 4-h shifts/week; structural and elemental microanalysis; minimum probe diameter <10 nm
JEOL 120C Transmission Electron Microscope	TEM resolution ~0.34 nm; special polepiece for TEM of ferromagnetic materials	120 kV; ten 4-h shifts/week; structural microanalysis
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam size; fracture stage; residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies
Varian Scanning Auger Electron Spectroscopy System	5 μm beam size; hot-cold fracture stage; residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Dual Ion-Beam Accelerator Facilities	4 MW Van de Graaff accelerator; 400 kV accelerator; sputter depth profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis
Philips EM430T Analytical Electron Microscope	300 kV, STEM, EDS, EELS	To be delivered late FY 1984
Atom Probe/Imaging Atom Probe/Field Ionization Microscope	Atomic resolution imaging, single atom analysis	To be delivered FY 1985

CENTER FOR MICROANALYSIS OF MATERIALS

Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

The Center operates a wide range of advanced surface chemistry and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, microcrystal-lography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded by MRL contracts of U of Illinois faculty, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative rsearch through a contract with a faculty member associated with the MRL, or by direct negotiation with the management of the Center. Direct user access to the equipment is also possible, for trained individuals. In all cases, the research carried out by facility users has to be in the furtherance of DOE objectives.

The facility staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

A brochure describing the Center and its services is available.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217)-333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

CENTER FOR MICROANALYSIS OF MATERIALS

Instruments	Features and Charactersitcs
Imaging Secondary Ion Microprobe Cameca IMS 3f	Dual ion sources (C_s^+,O_2^+). Depth profiling and mass analyzed secondary ion images with 1μm resolution.
Scanning Auger Microprobe Physical Electronics 595	Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector.
Scanning Auger Micropobe Physical Electronics 545	Resolution: SEM 3μm.
XPS Physical Electronics 548	Double pass CMA. ESCA and Auger. Specimen temp. to 1550K.
Transmission Electron Microscope Philips EM430 (300kV)	Delivery June 1984, EDS, EELS.
Transmission Electron Microscope Philips EM420 (120kV)	EDS. Cold stage (30K). Computer Control.
Transmission Electron Microscope Philips EM400T (120kV)	EDS. Heating, cooling stages.
Scanning Transmission Electron Microscope Vacuum Generators HB 5 (100kV)	0.5 nm probe, field emission gun, EDS, EELS.
Scanning Electron Microscope JEOL JSM 35C (35kV)	5 nm resolution, EDX, channelling and backscattering patterns.
Rutherford Backscattering (in-house construction) (3 MeV)	Two work stations, channelling
X-ray Equipment Elliott 14 kW high brilliance source Rigaku 12 kW source Several Conventional Sources	4-circle diffactometer. Small angle camera. EXAFS. Lang topography. Powder cameras, etc.

In addition to the main items listed above the Center also has other equipment: an electron microprobe, a spark-source mass spectrometer, optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including five ion-milling stations, evaporators, electropolishing units, sputter coaters, a spark cutter, ultrasonic cutter, diamond saw, dimpler, etc.

The equipment is made available on a flexible week-by-week booking scheme; if professional help is required, operating hours are 8-5, except by special arrangement. Fully qualified users can and do use the equipment at any time of day. Several of the instruments are maintained in almost continuous (24 hour) use.

D-21

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

This program utilizes a new approach for fundamental materials research. The combined techniques of ion implantation doping, ion-induced mixing, and pulsed-laser processing are utilized to alter the near-surface properties of a wide range of solids in ultrahigh vacuum. Through in situ analysis by ion beam, surface, and bulk properties techniques, the fundamental materials interactions leading to these property changes are determined. Since both ion implantation doping and pulsed-laser annealing are nonequilibrium processing techniques, they can be used to produce new and often unique materials properties not possible with equilibrium fabrication techniques. This makes them ideal tools for fundamental materials research. They are equally useful for modifying surface properties for practical applications in areas such as friction, wear, corrosion, catalysis, surface hardness, solar cells, semiconducting devices, superconductors, etc.

This program has emphasis on long-range basic research. Consequently, most collaborative research involving scientists from industries, universities, and other laboratories has been the investigation of new materials properties possible with these processing techniques or the determination of the mechanisms responsible for observed property changes. In most instances such research projects identify definite practical applications and accelerate the transfer of these materials alteration techniques to processing applications.

COLLABORATIVE RESEARCH

User interactions are through mutually agreeable collaborative research projects between users and research scientists at ORNL which utilize the unique alteration/analysis capabilities of the SMAC facility. Because of the tremendous interests expressed in these techniques and the broad range of existing collaborations, plans for a users' facility have been initiated. Until this program has been established, the informal arrangement will be continued. It should be emphasized that the goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application and not to provide routine service alterations or analyses.

PERSON TO CONTACT FOR INFORMATION

B. R. Appleton (615) 574-6283
Solid State Division FTS 624-6283
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

TECHNICAL DATA

Accelerators	Operating Characteristics
2.5-MV Positive Ion Van de Graaff	0.1–3.2 MeV; H, D, ^{4}He, ^{3}He, and selected gases. Beam current $\sim$50 μamps.
1.7-MV Tandem	0.2–3.5 MeV H; 0.2–5.1 MeV ^{3}He, ^{4}He; negative ion sputtering source for heavy ion beams of most species to 7 MeV.
10–200-KV High-Current Ion Implantation Accelerator	Essentially any species of ion. 1–3 mamps singly charged, $\sim$100 μamps doubly and triply charged.
0.1–10-KeV Ion Gun	Gaseous species. $\sim$20 μamps.
Lasers	
Pulsed Ruby Laser (0.6943 μm)	15–30 x 10^{-9} s pulse duration time. 10 Joule/Pulse Output Multimode, 2 Joule/Pulse Output Single Mode (TEM$_{oo}$).
Pulsed Ruby Laser (0.6943 μm)	15–30 x 10^{-9} s pulse duration time. 8 Joule/Pulse Output Single Mode (TEM$_{oo}$).
Pulsed Excimer Laser (0.249 μm)	20 x 10^{-9} s. 1.0 Joule/Pulse.
Facilities	
UHV Surface and Near-Surface Analysis Chambers	Several chambers. Vacuums 10^{-6}–10^{-11} Torr. Multiple access ports. Liquid helium cryostat, UHV goniometers (4–1300 K).
In Situ Analysis Capabilities	Ion scattering, ion channeling, ion-induced nuclear reactions and characteristic X rays. LEED, Auger, ion-induced Auger. Laser fluorescence spectroscopy. Electrical resistivity vs temperature.
Combined Ion-Beam and Laser Processing	Laser and ion beams integrated into same UHV chambers.
Dual Simultaneous Ion-Beam Irradiations	Combined accelerator irradiations.

D-23

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94550

Optical techniques, primarily spontaneous Raman spectroscopy, are being developed and used to study high-temperature corrosion and erosion of materials exposed to combustion environments. Emphasis is on the use of these techniques to identify chemical compounds present on surfaces during attack and the resultant effects on structural phase of the material under study. In situ analyses can be obtained with good temporal resolution (approximately ten spectra per second) for samples in high-temperature corrosive environments. Both pulsed and continuous-wave lasers at various wavelengths throughout the visible and ultraviolet regions are available for excitation of Raman scattering, which can be detected with photon counting, gated integration, or optical multichannel techniques. Samples can be exposed to high-temperature corrosive environments in laboratory furnaces, which have optical access for in situ measurements. These experiments can likewise be performed with 1-2 micron resolution on a Raman microprobe, which has a hot stage for in situ studies. Also available is the Atmospheric Combustor Exhaust Simulator, which is instrumented for Raman spectroscopy and provides a realistic environment for corrosion and erosion studies relevant to combustion systems. Real-time measurements are complemented by post-exposure techniques such as Raman spectroscopy with sputtering, scanning Auger spectroscopy, low-energy electron diffraction, x-ray diffraction, and metallographic analysis to provide additional compositional and morphological information.

USER MODE

The materials program at the Combustion Research Facility has emphasized research into corrosion and erosion mechanisms using the techniques and apparatus described above. Interactions include: (1) collaborative research projects with outside users, and (2) technology transfer of new diagnostic approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the person listed below. If further investigations appear reasonable, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government laboratories have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSON TO CONTACT FOR INFORMATION

Richard E. Palmer	(415) 422-3126
Division 8354	FTS 532-3126
Sandia National Laboratories	
Livermore, California 94550	

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

TECHNICAL DATA

Instruments	Key Features	Comments
Raman Surface Analysis System	UHV Chamber; Raman system with Ar laser, triple spectrograph and OMA; scanning Auger; sputtering capability.	Simultaneous Raman and sputtering. Raman system capable of detecting 22 nm thick oxides, up 10 spectra per second. Sample heating up to 1100C.
Raman Microprobe	Hot stage; Raman system with Ar , Kr lasers, scanning triple spectrometer.	1-2 micron spatial resolution. Hot stage can handle corrosive gases.
Raman High-Temperature Corrosion System	Furnace; Raman system with Ar , Kr , Cu-vapor lasers, triple spectrograph and OMA.	Cavity-dumped Ar laser and Cu-vapor laser allow gated detection for black-body background rejection. 50 micron x 2 mm spatial resolution. Sample heating up to 1000C. Up to 10 spectra per second.
Atmospheric Combustor Simulator	Raman system with Ar laser, scanning triple	Burns methane or fuel oil. 6 m/s flow. 1000C temperatures. Particulate and impurity gas injection.

D-25

MATERIALS PREPARATION CENTER

Ames Laboratory
Iowa State University
Ames, Iowa 50011

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section and the Materials Referral System and Hotline (MRSH). The Analytical Section has extensive expertise and capabilities for the characterization of materials, including complete facilities for chemical and spectrographic analyses, and selected services of this section are available to the research community. The purpose of MRSH is to accumulate information from all known National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community.

USER MODE

Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Frederick A. Schmidt, Director, Materials Preparation Center.

Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquires should be directed to Tom Wessels, MRSH Manager, (515) 294-8900 or FTS 865-8900.

TECHNICAL DATA

Materials

Scandium
Yttrium
Lanthanum
Cerium
Praseodymium
Neodymium
Samarium
Europium
Gadolinium
Terbium
Dysprosium
Holmium
Erbium
Thulium
Ytterbium
Lutetium

Titanium
Vanadium
Chromium
Manganese
Zirconium
Niobium
Molybdenum
Hafnium
Tantalum
Tungsten

Magnesium
Calcium
Strontium
Barium

Thorium
Uranium

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt, Director (515) 294-5236
Materials Preparation Center FTS 865-5236
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

CENTER FOR X-RAY OPTICS

Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

The Center for X-Ray Optics was created in August, 1983 to take the lead in developing new optical components and techniques for both science and industry. In the few months of its existence, the Center has begun to develop and use new technologies for the efficient transport, focusing, dispersion, and detection of radiation with photon energies extending from 20 eV to many keV, as well as the production of classical and coherent x-ray sources. Already established programs include microfabrication techniques, mirror technology, pulsed sources, and the development of coherent XUV radiation.

One major goal of the new Center is to provide a national resource for scientists working with radiation in the above spectral regions, including those at the various soft x-ray and VUV synchrotron radiation facilities. Specific plans include developmental work on reflective and diffractive optics, multilayer coatings for extending x-ray interference capabilities, picosecond x-ray detectors, developing a soft x-ray standards laboratory, and participation in undulator and high gain FEL experiments appropriate for this spectral region.

USER MODE

Collaboration with scientists active in this technical area.

PERSON TO CONTACT FOR INFORMATION

David Attwood
Center for X-Ray Optics
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

(415) 486-4463, or
FTS 451-4463

TECHNICAL DATA/FACILITIES

New laboratories and collaborations being organized.

NATIONAL CENTER FOR ELECTRON MICROSCOPY

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

The National Center for Electron Microscopy (NCEM) was formally established in fall 1981 as a component of the Materials and Molecular Research Division, Lawrence Berkeley Laboratory.

The NCEM provides unique facilities and advanced research programs in the United States for electron microscopy characterization of materials. Its mission is to carry out fundamental research and maintain state-of-the-art facilities and expertise. Present instrumentation at the Center includes a conventional 650 kV Hitachi electron microscope installed in 1969 in the Hearst Mining Building on the University of California Berkeley campus, and a 1.5 MeV Kratos microscope dedicated largely for in-situ work, a 1 MeV JEOL atomic resolution microscope (ARM), and a high-resolution feeder microscope (JEOL 200CX). A 200 kV analytical microscope was recently installed. Facilities for image simulation, analysis, and interpretation are also available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. J. J. Hren, Chairman; W. L. Bell, J. M. Gibson, D. A. Howitt, A. Simnad, J. C. H. Spence, and A. Taylor; internal members are G. Thomas, T. L. Hayes, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be of sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore
National Center for Electron Microscopy
Mail Stop: 72-131
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

(415) 486-6062, or
FTS 451-6062

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characterization
KRATOS 1.5 MeV Electron Microscope	Resolution 3Å (pt-pt) environmental cell; hot, cold stages	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. Max beam current 70 amp/cm^2. 3 mm diameter specimens
JEOL 1 MeV Atomic Resolution Microscope	Resolution $\leq$ 1.7Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, ± 40° biaxial tilt with height control	50-80 hrs/week, 400 kV - 1 MeV, LaB$_6$ filament, 3 mm diameter specimens
Hitachi 650 kV Electron Microscope	General purpose resolution 20 Å environmental cell straining stage	Installed in 1969. Max. voltage 650 kV conventional HVE
JEOL 200 CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only	200 kV only, LaB$_6$ filament, 2.3 mm diameter specimens
200 kV dedicated Analytical Electron Microscope	X-ray and energy-loss spectrometers micro-diffraction (CEB)	100 kV - 200 kV LaB$_6$ filament, state-of-the-art resolution

SECTION E

Summary of Funding Levels

SUMMARY OF FUNDING LEVELS

During the fiscal year ending September 30, 1984, the Materials Sciences total support level amounted to about $125.1 million in operating funds (budget outlays) and $12.7 million in equipment funds. The following analysis of costs is concerned only with operating funds (including SBIR) i.e., equipment funds which are expended primarily at Laboratories are not shown in the analysis. In contrast, equipment support for the Contract and Grant Research projects is included as part of the operating budget.

1. By Region of the Country:

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Northeast............... (CT, DC, DL, MA, MD, ME, NJ, NH, NY, PA, RI, VT)	47.3	26.4
(b) South................... (AB, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	8.2	18.7
(c) Midwest................. (IA, IL, IN, MI, MN, MO, OH, WI)	23.2	29.7
(d) West.................... (AZ, CO, KS, MT, NB, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	21.3	25.2
	100.0	100.0

2. By Discipline:

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-)	60.0	39.0
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	33.0	50.3

SUMMARY OF
FUNDING LEVELS

	Contract and Grant Research (% by $)	Total Program (% by $)
(c) Chemistry, Chemical Eng. (Budget Activity Numbers 03-)	6.7	10.7
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including laboratories where graduate students are involved in research to a large extent, i.e., LBL, Ames and IL)...	36.8
(b) DOE Laboratory Programs...........	62.0
(c) Industry and Other................	1.2
	100.0

4. By Laboratory and Contract and Grant Research

	Total Program (%)
Ames Laboratory	6.0
Argonne National Laboratory	16.8
Brookhaven National Laboratory	18.3
Idaho National Engineering Laboratory	0.4
Illinois, University of (Materials Research Laboratory)	2.6
Lawrence Berkeley Laboratory	10.6
Lawrence Livermore National Laboratory	1.2
Los Alamos National Laboratory	3.1
Oak Ridge National Laboratory	16.8
Pacific Northwest Laboratory	1.6
Sandia National Laboratories	3.3
Solar Energy Research Institute	0.3
Stanford Synchrotron Radiation Laboratory	0.6
Contract and Grant Research	18.4
	100.0

SUMMARY OF
FUNDING LEVELS

5. By Selected Areas of Research:

	% of Prorated Projects[a] (Total=415)	% of Program Funding[a] ($125.1 million)	% of Individual Projects[c] (Total=415)
Materials			
Ceramics (Crystalline)	18.0	15.0	25.0
Ferrous Alloys	6.2	3.9	17.3
Intermetallics	3.9	3.3	9.4
Polymers	4.1	2.4	6.2
Semiconductors	8.2	7.2	13.0
Technique			
Electron Microscopy (Technique Development)	3.2	2.8	7.2
Neutron Scattering	4.7	17.8	9.2
Synchrotron Radiation	3.0	10.3	5.1
Theory	14.0	11.2	37.6
Phenomena			
Catalysis	2.7	2.8	6.7
Corrosion	6.1	4.5	10.4
Diffusion	5.8	4.2	14.2
Processing Science/Synthesis[b]	16.1	12.3	29.6
Strength	9.3	4.8	16.1
Superconductivity	3.8	3.7	6.3
Environment			
High Temperature (> 1200°K)	4.4	4.0	6.3
Radiation	5.1	11.4	9.0
Sulfur-Containing Gases	1.5	1.3	2.9

[a] The funding levels and projects percentage for various research categories were determined from the index listing in Section F and estimating the percentage from the project devoted to a particular subject. There is overlap in the figures. For instance, funding for a project addressing creep of oxides would appear in the categories of ceramics, strength, and (possibly) high temperature.

[b] Based on projects indexed in Section F under coatings, materials, preparation, powder metallurgy, solidification, surface treatments, thin films, and welding.

[c] Percentage of sum of individual projects involving the designated area of materials research.

SECTION F

Index of Investigators, Materials, Techniques, Phenomena and Environment

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011, 026, 041, 044, 045, 074, 081, 109, 119, 144, 151, 156, 163, 169, 170, 171, 219, 225, 233, 235, 239, 243, 248, 260, 267, 290, 293, 295, 302, 304, 305, 315, 324, 327, 333, 339, 340, 348, 362, 363, 368, 369, 370, 371, 372, 373, 374, 375, 379, 386, 390, 396, 397, 407, 410, 411, 412, 427, 429, 430, 437, 445, 446, 450, 452, 457, 460, 465, 468, 483, 486

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024, 045, 081, 118, 144, 148, 151, 153, 159, 233, 235, 239, 260, 265, 290, 293, 315, 330, 333, 339, 351, 363, 373, 374, 390, 397, 410, 411, 412, 424, 430, 443, 465, 471, 479, 504

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Platinum Metal Alloys (Platinum, Palladium, Rhodium, Irridium, Osmium, Ruthenium
003, 029, 074, 131, 142, 149, 169, 173, 177, 318, 388, 431, 455, 460, 463, 475

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047, 078, 130, 164, 167, 204, 205, 206, 312, 320, 323, 324, 329, 347, 357, 378, 388, 416

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001, 003, 006, 007, 009, 012, 013, 016, 017, 018, 020, 023, 024, 025, 026, 027, 050, 076, 077, 081, 167, 193, 227, 229, 239, 244, 266, 337, 388, 391, 416, 439, 441, 461, 484, 489

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004, 005, 007, 008, 012, 018, 028, 040, 042, 073, 080, 113, 140, 168, 173, 191, 235, 238, 303, 352, 402, 456, 514

Semiconductor Materials - Elemental (including amorphous phases)
014, 019, 060, 070, 080, 121, 123, 124, 140, 160, 161, 162, 163, 166, 176, 177, 194, 231, 238, 241, 243, 261, 267, 275, 319, 338, 339, 356, 366, 392, 400, 401, 402, 435, 457, 461, 472, 494, 512

Semiconductor Materials - Multicomponent (III-Vs, II-VIs and amorphous forms)
014, 016, 019, 051, 108, 120, 123, 124, 125, 132, 152, 160, 161, 194, 231, 243, 261, 277, 296, 310, 339, 366, 386, 400, 401, 410, 415, 445, 471, 480, 494

Solid Electrolytes (see also fast ion conductors)
025, 051, 054, 078, 081, 121, 129, 234, 235, 301, 333, 412, 436, 444, 448, 486

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011, 026, 027, 112, 114, 116, 117, 119, 141, 148, 177, 201, 202, 207
219, 225, 226, 246, 290, 304, 327, 343, 363, 370, 375, 379, 383, 410
437, 457, 459, 468, 472, 501, 502, 503, 511

Superconductors (also see Superconductivity in the Phenomena index and Theory in the Techniques index)
004, 013, 015, 019, 022, 047, 048, 050, 053, 055, 056, 072, 075, 077
127, 147, 164, 166, 167, 228, 230, 279, 303, 318, 350, 378, 380, 389
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147, 149, 159, 203, 218, 222, 224, 241, 262, 263, 278, 293, 295, 303
318, 319, 351, 367, 372, 382, 384, 404, 475, 483, 491

Bulk Analysis Methods (other than those listed separately in this index, e.g., ENDOR, muon spin rotation, etc.)
007, 008, 012, 042, 200, 230, 374, 478

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006, 022, 026, 041, 054, 057, 058, 071, 147, 162, 164, 165, 166, 173
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313, 322, 323, 329, 333, 336, 339, 354, 355, 356, 367, 368, 375, 381
389, 412, 426, 432, 448, 450, 460, 468, 469, 471, 477, 488

Chemical Vapor Deposition (all types)
070, 277, 280, 385, 466

Deep Level Transient Spectroscopy
415, 441, 494

Electron Diffraction (Technique development, not usage, for all types--LEED, RHEED, etc.)
053, 106, 107, 108, 109, 112, 241, 278, 302, 317, 367, 414, 456, 475
493

Electron Energy Loss Spectroscopy (EELS)
001, 014, 029, 044, 053, 070, 074, 106, 107, 112, 117, 140, 141, 217
241, 278, 302, 313, 316, 317, 333, 359, 362, 363, 383, 449, 471, 478
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006, 029, 057, 059, 074, 105, 125, 126, 168, 169, 172, 176, 234, 246
247, 260, 262, 279, 280, 292, 326, 332, 335, 365, 374, 382, 384, 386
409, 420, 453, 462, 465, 477, 513

Electron Microscopy (technique development for all types)
002, 003, 004, 005, 041, 042, 043, 044, 045, 106, 107, 109, 110, 111
112, 114, 116, 117, 120, 140, 141, 142, 143, 144, 146, 147, 149, 155
190, 201, 217, 224, 231, 232, 238, 260, 263, 302, 338, 340, 352, 363
368, 394, 411, 414, 419, 422, 447, 457

Electron Spectroscopy for Chemical Analysis (ESCA)
058, 059, 108, 194, 262, 263, 440, 483

Electron Spin Resonance or Electron Paramagnetic Resonance
017, 121, 239, 279, 344, 390, 397, 452, 461, 465

Extended X-Ray Absorption Fine Structure (EXAFS and XANES)
023, 052, 059, 060, 071, 072, 073, 074, 106, 118, 127, 168, 169, 176
200, 264, 278, 305, 311, 333, 371, 394, 397, 398, 403, 404, 409, 411
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Field Emission and Field Ion Microscopy
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014, 043, 060, 108, 200, 280, 291, 292, 319, 352, 377, 414, 456, 515

Ion Channeling, or Ion Scattering (including Rutherford and other ion scattering methods)
040, 043, 044, 106, 203, 226, 239, 242, 243, 247, 264, 295, 303, 319
362, 491

Internal Friction (also see Ultrasonic Testing and Wave Propagation)
005, 007, 008, 075, 111, 113, 128, 333, 444

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014, 025, 051, 058, 070, 160, 231, 233, 234, 261, 295, 310, 350, 361
371, 394, 398, 408, 412, 426, 442, 444

Laser Spectroscopy (scattering and diagnostics)
100, 126, 161, 163, 194, 231, 267, 280, 290, 293, 295, 306, 310, 321
324, 332, 337, 363, 385, 392, 394, 395, 399, 408, 414, 438, 443, 453
466, 472, 477, 486, 492, 494

Magnetic Susceptibility
002, 009, 010, 017, 050, 127, 154, 165, 230, 279, 318, 371, 378, 400
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053, 108, 123, 277

Mossbauer Spectroscopy
025, 239, 264, 311, 361, 393

Neutron Scattering: Elastic (Diffraction)
018, 023, 047, 048, 049, 057, 076, 077, 078, 081, 084, 113, 130, 132
204, 227, 228, 229, 245, 318, 333, 347, 376, 391, 394, 411, 416

Neutron Scattering: Inelastic
008, 018, 047, 049, 057, 073, 076, 077, 078, 084, 130, 132, 154, 204
227, 228, 229, 347, 361, 391, 394, 410, 425

Neutron Scattering: Small Angle
047, 049, 084, 132, 172, 218, 228, 230, 245, 311, 364, 394, 413, 468

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017, 018, 060, 131, 162, 174, 177, 264, 279, 311, 312, 388, 412, 436
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070, 125, 126, 277, 344, 395, 409

Positron Annihilation (including slow positrons)
040, 075, 080, 291

Powder Consolidation (including sintering, hot pressing, dynamic compaction, laser assisted, etc., of metals and ceramics, see also this item in the Phenomena index)
011, 119, 148, 150, 153, 156, 192, 202, 225, 244, 343, 450

Powder Synthesis (including preparation, characterization, or pre-consolidation behavior, see also this item in the Phenomena index)
011, 046, 072, 081, 119, 148, 153, 156, 202, 225, 378, 450

Raman Spectroscopy (also see Infrared Spectroscopy)
053, 059, 127, 205, 234, 246, 261, 264, 265, 267, 277, 280, 290, 293
311, 316, 324, 361, 363, 371, 377, 386, 412, 425, 452, 453, 480, 486

Rapid Solidification Processing (also see Solidification: Rapid in the Phenomena index)
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001, 005, 011, 029, 060, 080, 106, 108, 113, 126, 161, 194, 242, 261
264, 276, 316, 318, 359, 374, 404, 456, 463, 483

Specific Heat
009, 018, 052, 127, 279, 311, 312, 357, 416

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001, 002, 043, 053, 055, 060, 078, 081, 108, 171, 244, 261, 263, 266
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085, 175, 177, 216, 305, 330, 340, 368, 394, 398, 402, 403, 404, 409
411, 414, 439, 441, 445, 460, 474, 298

Surface Treatments (including ion implantation, laser processing, electron beam processing, sputtering, etc., see Chemical Vapor Deposition)
014, 040, 043, 044, 080, 083, 105, 107, 110, 156, 159, 190, 191, 226
231, 233, 239, 242, 243, 247, 265, 266, 267, 277, 319, 359, 369, 373
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010, 056, 207

Theory: Surface
020, 021, 029, 054, 082, 151, 173, 176, 237, 276, 278, 280, 317, 355
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Theory: Structural Behavior
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426, 432, 433, 434, 454, 470, 472, 476, 480, 488, 489

Theory: Superconductivity
022, 054, 082, 164, 323, 354, 440, 484

Theory: Thermodynamics, Statistical Mechanics, and Critical Phenomena
006, 054, 057, 058, 059, 082, 130, 142, 148, 174, 205, 206, 208, 215
231, 237, 245, 246, 248, 276, 312, 322, 323, 325, 329, 347, 355, 358
384, 389, 417, 448, 454, 455, 457

Theory: Transport, Kinetics, Diffusion
003, 004, 007, 008, 026, 027, 040, 041, 046, 051, 054, 082, 105, 124
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010, 100, 105, 113, 128, 207, 308, 423, 472, 473

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008, 016, 085, 176, 338, 361, 369, 394, 404, 409, 441

X-Ray Scattering and Diffraction (wide angle crystallography)
002, 019, 023, 024, 026, 027, 028, 048, 073, 079, 081, 085, 106, 113
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079, 085, 106, 118, 154, 176, 221, 236, 245, 276, 311, 394, 403

X-Ray Scattering (other than crystallography)
019, 047, 085, 106, 176, 216, 340, 362, 394, 445, 447, 490

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008, 018, 024, 025, 052, 074, 085, 106, 176, 203, 241, 262, 264, 278
295, 351, 394, 411, 426, 439, 471, 474, 478

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016, 046, 155, 164, 171, 176, 244, 266, 267, 276, 280, 290, 396, 398
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015, 024, 056, 070, 079, 120, 125, 131, 152, 233, 240, 261, 277, 279
296, 303, 310, 323, 356, 366, 369, 392, 400, 401, 411, 414, 435, 443
452, 465, 471, 480, 491

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025, 041, 051, 120, 233, 234, 301, 333, 369, 377, 390, 412, 436, 444
448, 465, 486

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010, 059, 071, 105, 247, 262, 264, 265, 326, 365, 382, 384, 386, 420
451, 453, 462, 513, 515

Corrosion: Gaseous (e.g., oxidation, sulfidation, etc.)
045, 071, 144, 153, 155, 158, 159, 170, 220, 263, 290, 293, 302, 316
318, 351, 358, 359, 372, 386, 409, 422, 437, 452

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076, 077, 079, 084, 276, 312, 322, 329, 332, 347, 354, 367, 388, 393
399, 400, 410, 438, 454, 474, 476, 487

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017, 023, 024, 025, 027, 028, 044, 048, 049, 076, 077, 079, 081, 084
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007, 008, 012, 018, 027, 040, 041, 054, 105, 113, 129, 132, 145, 170
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045, 072, 168, 172, 234, 311, 319, 322, 343, 352, 368, 369, 372, 401
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005, 042, 114, 117, 122, 142, 201, 218, 232, 265, 291, 296, 302, 308
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002, 008, 016, 017, 018, 020, 021, 024, 028, 048, 050, 052, 053, 054
058, 078, 080, 083, 123, 127, 131, 152, 165, 203, 215, 233, 237, 311
318, 366, 404, 409, 417, 439, 440, 441, 453, 456, 461, 474, 478, 484
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014, 016, 021, 025, 052, 058, 080, 108, 121, 123, 125, 163, 165, 166
174, 194, 237, 296, 310, 323, 330, 337, 344, 366, 390, 392, 400, 401
411, 415, 435, 443, 454, 477, 483, 485, 486, 492, 494

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003, 005, 041, 045, 055, 059, 071, 072, 109, 116, 119, 140, 148, 156
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059, 112, 114, 116, 158, 275, 382, 404, 421

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009, 020, 047, 049, 050, 053, 076, 079, 084, 121, 127, 146, 167, 174
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043, 116, 117, 150, 218, 307, 314, 331, 334, 341, 364, 383, 413, 434
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Mechanical Properties and Behavior: Fatigue
010, 114, 232, 307, 309, 331, 334, 365, 387, 406, 413, 419, 434, 458
469, 473, 482, 514

Mechanical Properties and Behavior: Flow Stress
005, 010, 041, 117, 201, 219, 291, 308, 341, 342, 345, 346, 370, 381
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005, 010, 100, 114, 116, 117, 141, 147, 148, 149, 159, 200, 201, 202
203, 218, 219, 232, 291, 304, 307, 309, 326, 334, 342, 345, 346, 349
360, 364, 379, 382, 383, 387, 406, 407, 419, 422, 429, 433, 457, 458
469, 472, 481, 511

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011, 026, 027, 081, 112, 116, 119, 120, 141, 143, 148, 150, 156, 177
202, 207, 225, 235, 236, 246, 266, 267, 276, 304, 315, 327, 330, 339
343, 344, 348, 363, 371, 374, 375, 383, 390, 397, 398, 408, 412, 424
426, 430, 444, 450, 459, 460, 465, 466, 479, 492, 501, 502, 503, 504

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002, 004, 012, 015, 017, 024, 048, 050, 053, 100, 127, 141, 142, 143
145, 147, 168, 169, 171, 172, 190, 191, 192, 203, 207, 235, 236, 244
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014, 024, 051, 070, 123, 143, 152, 177, 235, 277, 296, 319, 356, 377
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315, 325, 327, 363, 369, 373, 374, 375, 381, 384, 413, 421, 426, 459
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291, 306, 308, 333, 344, 352, 368, 408, 411, 415, 427, 448, 455, 462
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011, 026, 046, 107, 119, 150, 153, 156, 192, 202, 315, 343, 344, 369
374, 375, 383, 408, 430, 450, 459, 465, 479, 501, 503, 505, 507

Powder Synthesis (including preparation, characterization, or pre-consolidation behavior, see same item under Technique index)
011, 027, 107, 119, 153, 156, 202, 246, 249, 276, 315, 343, 374, 375
378, 430, 450, 459, 502, 503, 504

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040, 042, 043, 060, 075, 222, 238, 240, 265, 295, 392, 458

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010, 047, 200, 207, 261, 396, 472, 473

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001, 010, 059, 071, 105, 149, 247, 262, 278, 382, 384, 386, 420, 451
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002, 003, 107, 110, 190, 191, 192, 221, 237, 242, 311, 322, 345, 371
372, 380, 467, 491, 502, 508

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172, 173, 203, 204, 241, 262, 280, 302, 316, 317, 355, 357, 367, 374
385, 386, 403, 404, 405, 431, 449, 456, 463, 483, 493

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021, 083, 085, 262, 312, 316, 385, 431, 449

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020, 021, 029, 058, 074, 085, 131, 165, 237, 241, 242, 262, 278, 302
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357, 381, 383, 390, 424, 426, 439, 447, 454, 455, 457, 476, 480, 484

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Summaries of FY 1984 Research in the Chemical Sciences

September 1984

U.S. Department of Energy
Office of Energy Research
Division of Chemical Sciences

This report was compiled for the Office of Energy Research project from summaries contained in the Research-In-Progress (RIP) data base of the Office of Scientific and Technical Information, Oak Ridge, Tennessee. The RIP data base describes new and ongoing energy and energy-related research projects carried out or sponsored by the Department of Energy.

PREFACE

The purpose of this publication is to inform those interested in research supported by the Department of Energy's Division of Chemical Sciences, which is one of six Divisions of the Office of Basic Energy Sciences in the Office of Energy Research. This year, for the first time, this publication shows projects supported by that portion of the Nuclear Sciences budget which is administered by the Division of Chemical Sciences.

These summaries provide to members of the scientific and technical public and interested persons in the legislative and executive branches of the Government a means for becoming acquainted, either generally or in some depth, with the Chemical Sciences program. Areas of research supported by the Division are to be seen in the section headings, the index, and the summaries themselves. Energy technologies that can be advanced by use of the basic knowledge generated in this program are provided in the index and also (by reference) in the summaries.

Chemists, physicists, chemical engineers, and others who are considering the possibility of proposing research for support by this Division will find the publication useful for gauging the scope of the present program in basic research and the relationship of their interests to the overall program. Proposals that expand this scope will also be considered or directed to more appropriate offices. The research summarized here is intended to add significantly to the knowledge base on which successful energy technologies can grow. For this purpose, scientific excellence is a major criterion applied in the selection of research supported by the Division of Chemical Sciences. Another important consideration is the emphasizing of chemical, physical, and chemical engineering subdisciplines which are advancing in ways that produce new information related to energy, needed energy data, or new ideas.

The program is distributed among several different kinds of performing organizations. About half the projects take place at DOE laboratories, and half take place at universities and industrial laboratories. In DOE laboratories, most of the researchers are fully engaged in this work, whereas most university and industrial researchers necessarily divide their time among duties involving this research, other research, teaching responsibilities, etc. Thus about 70% of the funding goes to Federal laboratories, 25% to the academic sector, and the remainder to industrial and nonprofit laboratories.

Questions about the details of an individual project may be directed to the investigators involved or the persons in charge at DOE Laboratories (who are identified at appropriate places in this publication). Other questions about the program may be directed to the undersigned.

Elliot S. Pierce, Director
Division of Chemical Sciences
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[*] On leave from Lehigh University.

[†] On leave from Brigham Young University.

Each Branch of the Division of Chemical Sciences is divided into programs which cover various disciplines. The following summaries describe these programs. The staff members responsible for each program are indicated on page ii.

Fundamental Interactions Branch (01-   )

Photochemical and Radiation Sciences (01-01)

The Photochemical and Radiation Sciences program consists of research into the interactions of radiation with matter in all forms but particularly with gases and liquids. The photochemical research is devoted largely to studies with visible radiation aimed at the capture and conversion of solar energy. This encompasses such fields as artificial photosynthesis, photoinduced electron transfer reactions in homogeneous and heterogeneous media, photoelectrochemistry, and photocatalysis. The radiation chemistry research is concerned with the chemical effects produced by absorption of energy from ionizing radiation. A small part of the program is devoted to research in hot atom chemistry, i.e., the study of the effects of nuclear decay and the consequent release of energy on chemical reactions. A new and growing program of photochemistry, spectroscopy, and related studies is centered at the National Synchrotron Light Source at Brookhaven National Laboratory.

Chemical Physics (01-02)

The Chemical Physics program supports research in a diverse set of disciplines with a goal of providing basic knowledge in areas related to the nation's energy needs. A significant portion of the program is in the many-faceted area of chemical kinetics, including energy transfer, chemical dynamics involving state-selected chemistry, unimolecular and biomolecular research kinetics, as well as the reactions of clusters. Research efforts in molecular structure, spectroscopy, and theoretical chemistry are also well represented in this program.

Special emphasis is placed on basic research related to combustion; advanced diagnostic methods, spectroscopy, theory, and the kinetics of elementary combustion reactions are of special interest. A major user-oriented facility, the Combustion Research Facility (CRF) at Sandia Laboratories/Livermore is supported by this program. This laboratory offers use of advanced instrumentation to interested combustion scientists from universities, industry, and national laboratories.

Atomic Physics (01-03)

The Atomic Physics program supports experimental and theoretical efforts associated with the study of atom and ion structures, energy levels and lifetimes of quantum states, and of transport and exchange processes characterizing transfer of energy, momentum, and matter. These studies strive to obtain the best and most complete fundamental knowledge of the properties and interactions of photons, electrons, atoms, ions, and simple molecules. Continued emphasis of this research has been on the understanding of relatively high energy atomic physics that involves atoms stripped of all or most all electrons and of atoms and ions in which electrons are located at upper energy levels. The study of processes that lead to the production of coherent radiation and of the statistical properties of this radiation as they modify elementary atomic physics processes also constitute part of this program.

Processes and Techniques Branch (02-   )

Chemical Energy (02-01)

This program includes basic chemistry research related to chemical transformations or conversions which are fundamental to new or existing concepts of energy production and storage. Of particular interest are those research activities with the objectives of understanding the chemical aspects of (1) catalysis, both heterogeneous and homogeneous, (2) the chemistry of fossil resources, particularly coal, including characterization and transformation, and (3) the conversion of biomass and related cellulosic wastes. The disciplines of organic, bio-, inorganic, physical, thermo-, and electrochemistry are central to this program. The emphasis is on understanding the chemical principles underlying the new and developing technologies and on innovative chemical research with potential for new energy concepts.

Separations and Analysis (02-02)

The separations part of the program is directed toward improving our basic understanding of methods for separating mixtures of gases, liquids, solids, and their component molecules, cations, anions, and isotopes. The program covers a broad spectrum of separations concepts, including membrane processes, extraction at both standard and supercritical conditions, adsorption, chromatography, photodissociation, complexation, etc. The program is technique oriented rather than species oriented; i.e., the research involves elucidating fundamental chemical phenomena for improved separations rather than developing specific processes for the separation of a particular species from particular matrices. The isotope separation program emphasizes isotopic properties and isotope effects and is basic in nature.

The analysis part of the program is aimed at supporting research on analytical techniques where a better understanding of basic chemical phenomena may facilitate improvements in sensitivity, reliability, and ease of operation and/or lower the costs of analytical determinations. Entirely new analytical techniques are also investigated, although this program does not support instrument development. New techniques are quickly reported in the literature so that those interested in instrument development can build on work supported herein. The program is not geared to using existing techniques to unravel the composition of samples nor to developing techniques to analyze particular chemical species or sample types. Rather, it is aimed at obtaining a thorough understanding of the basic chemistry of an analytical technique so that others may use this understanding to improve its utility.

Chemical Engineering Sciences (02-04)

This program addresses the more specific and energy-related aspects of chemically related engineering topics, including thermodynamics and physical and chemical rate processes. Particular attention is given to turbulence research related to combustion; experimental and theoretical thermochemical and thermophysical properties, and phase equilibria, especially of mixtures, including supercritical phenomena. Emphasis is given to improving and/or developing the scientific base for engineering generalizations and their unifying theories.

Isotope Preparations (KC-01-02)

The Isotope Preparations program is dedicated to the production of research quantities of isotopically enriched research materials by way of the Electromagnetic Isotope Separations (Calutron) facility, the High Flux Isotope Reactor (HFIR), and the Transplutonium Processing Plant (TRU). These facilities are described on pages 88 and 89 of this book. These research materials are made available to an international user community from a sales inventory, by loan from a Research Materials Collection, and by cost-free allocation from the DOE Research Materials/Transplutonium Program Committee.

Heavy Element Chemistry (KC-01-02-03)

The Heavy Element Chemistry program focuses on a study of the chemical and certain physical properties of the actinide elements, principally the transuranium elements, because of the importance of these elements to the DOE Nuclear Energy Technology program and to an understanding of the basic science in general. A variety of investigations are pursued, including (1) organometallic chemistry, (2) the chemistry of excited spectroscopic states, (3) thermochemistry of actinides in complex oxides and binary halides, (4) the chemistry of actinides in near-neutral aqueous solutions and the reactions of aqueous actinides ions with various complexing agents, (5) the development of preparative methods for actinide metals and compounds, and (6) the measurement of crystal structures melting point magnetic susceptibilities and the behavior of actinide metals under pressure. This research is performed principally at the National Laboratories because of facilities required for handling radioactivity.

LABORATORY ADMINISTRATION

Listed below, by laboratory and department or division, are persons who are in charge of the Division of Chemical Sciences projects at DOE laboratories. These individuals are laboratory, department, or division administrators who can provide information about specific programs or refer inquiries to appropriate individuals.

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NATIONAL LABORATORIES

Heavy Element Chemistry

Argonne National Laboratory
Argonne, Illinois 60439

Division of Chemistry **$1,300,000**

1. ***Heavy Element Chemistry Research***
W.T. Carnall, J.V. Beitz, H.M. Crosswhite, L.R. Morss, J.C. Sullivan

The objective of this program is to advance the chemistry and physics of the actinide elements consistent with the energy development goals of the Department of Energy. Laser spectroscopy and photophysics efforts explore and interpret the unique electronic structure of the actinides, while efforts in photochemistry and inorganic fluorine chemistry interact to develop novel processes for chemical and isotope separations utilizing high-valency reactive species of Np, Pu, and Am. Parallel research on Cm, Bk, Cf, and Es compounds extends the understanding of electronic structure and chemical properties of the heaviest elements. Solid state and organometallic research activities characterize new transuranium compounds, especially in low and high oxidation states, and systematize bonding and reactivity patterns throughout the series. Comparison with the chemistry of both the transition and rare earth elements is stressed, and emphasis is placed on the use of thermochemical methods. Oxidation-reduction and complex formation reactions of actinides in solution are investigated with pulse radiolysis, stopped-flow, NMR and thermodynamic methods in order to interpret and predict the behavior of these elements in modern process chemistry, as well as in the aqueous environment. [10.9 FTE]

Lawrence Berkeley Laboratory
Berkeley, California 94720

Materials and Molecular Research Division **$1,230,000**

2. ***Actinide Chemistry***
N.M. Edelstein

The purpose of this program is to study actinide materials in order to provide the basic knowledge necessary for their safe and economic utilization in present and future technology. The work includes the preparation of new gaseous, liquid, and solid phases and studies of their physical and chemical properties. Techniques for characterization include x-ray diffraction, optical and vibrational spectroscopy, magnetic resonance, and magnetic susceptibility. Equilibrium and kinetic data for complex formation are measured. From these complementary studies, new insights into the structural and chemical principles of actinide compounds are obtained with which to design new synthetic schemes to produce new materials. A major aspect of the program is the design and synthesis of sequestering agents for actinide ions. These compounds are intended for use in the treatment of actinide poisoning and for possible application in the treatment of spent reactor fuels. Preparative, structural, and physical studies of new types of organoactinide, related organolanthanide, and new actinide inorganic complexes are continuing. Studies on optical spectra of free ions and actinide ions in crystals are being pursued in order to understand their electronic structure. Applications of new spectroscopic techniques for characterization of actinide species in solution are being undertaken. [15.0 FTE]

Los Alamos National Laboratory
Los Alamos, New Mexico 87544

Isotope and Nuclear Chemistry Division **$260,000**

3. ***Actinide Valence, Host, and Radiation Effects***
P.G. Eller

There is only sparse information regarding valence stabilities of the transuranium elements Pu, Am, and Cm in solids important to nuclear waste storage. We are determining the effects of ion size and radiation on actinide valence stabilities and site selectivities, particularly of Am(III, IV) in selected oxide matrices. Since Pu, Am, and Cm have profoundly different aqueous valence stabilities, we anticipate stability differences when they are incorporated in solids and exposed to radiation (self radiation or other). We have developed an approach to predicting actinide valence stabilities and site selectivities in solids and are determining the validity of the hypothesis by synthesizing and studying appropriate actinide materials by spectroscopic and diffraction techniques. We also continue appropriate solid state and solution characterization of oxo and fluoride species (e.g.,

MO_2^+, MOF_6, and so forth). In addition to the obvious relevance to practical nuclear waste storage considerations, the work will also contribute to the general physico-chemical understanding of actinide behavior in condensed phase systems where oxygen is the coordinating ligand, either as free oxide ion, or when connected to another element (e.g., Si, P, and so forth). A major new initiative is exploring the applicability of Raman/resonance Raman techniques to the above materials. [0.9 FTE]

4. ***Actinide Chemistry in Near-Neutral Solutions***
T.W. Newton, D.E. Hobart

We are investigating a spectrophotometric method for determining the carbonate complexes of Pu(IV) and their association quotients. The method involves competition between citrate and carbonate ligands for the plutonium. Values for the formation quotients for the citrate complexes are available in the literature, but will be checked for applicability under our experimental conditions. The experiments are done on solutions saturated with argon containing known partial pressures of CO_2 in order to fix the thermodynamic activities of CO_2 and H_2CO_3. Preliminary experiments have shown that significant spectral changes occur when the pH is changed at constant citrate concentrations and when the citrate/bicarbonate ratio is changed at essentially constant pH. Measurements on solutions where each contains no citrate but has a different pH and constant CO_2 pressure indicate the presence of at least three carbonate-containing complexes in the pH range from 7 to 9.5. One or more of these may be hydroxo- or bicarbonato complexes. Spectral data are taken at 10 wavelengths between 400 and 700 nm. A non-linear least-squares program is being adapted for the quantitative interpretation of the data. [0.9 FTE]

Materials Science and Technology Division **$115,000**

5. ***Thermodynamics of the Transplutonium Elements and Early Actinides***
P.D. Kleinschmidt, J.W. Ward

Fundamental thermodynamic data are obtained on actinide elements, compounds, and alloys by using high temperature mass spectrometry and target collection techniques. The sublimation pressures of the pure metals actinium, protactinium, and promethium are being measured. The cohesive energy is derived from these numbers and is correlated with the electronic structure of these elements. From vapor composition measurements on the americium and protactinium oxides and plutonium fluorides, the entropy and enthalpy of sublimation are determined as well as the bond dissociation energies of the gas phase molecules. The actinide series is the only one in which f electrons participate in bonding, and the effect of this is to produce unique structures and compounds. These numbers will provide a data base for any study involving transplutonium elements and compounds. Fast breeder reactor technology will require such information, as will waste storage and disposal studies. [0.8 FTE]

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Chemistry Division **$1,225,000**

6. ***Chemistry of Transuranium Elements and Compounds***
O.L. Keller, C.E. Bamberger, G.M. Begun, J.K. Gibson, R.L. Hahn

The program emphasizes the role of 5f electrons and of relativistic effects in determining the chemical and physical behavior of the actinides. Fundamental studies include: (1) investigation of the changes in 5f bonding characteristics in actinide metals and compounds as a function of pressure (up to 57 GPa); (2) derivation of thermodynamic properties of metals and compounds from high temperature Knudsen cell/mass spectrometer measurements; and (3) the determination of hydration and complexation phenomena by neutron and (synchrotron) x-ray diffraction. Also, studies are conducted on high temperature synthesis of actinide compounds which may be of interest to their immobilization in solid crystalline hosts. A new direction is being developed as a result of recent renewed interest in proposed studies of the chemistry of element 103, Lr, the last of the 5f electron series, and of the transactinide elements, in which the 7s, 7p, and 6d electrons are important. These elements could be produced in relatively large yields at accelerators using an ~40 microgram target of ^{254}Es, if the necessary financial support is obtained. Currently, the chemical identification of Lr and the determination of the radius of the 3+ ion is being carried out on the basis of 20 atoms per bombardment using a 3μg ^{254}Es target. [10.4 FTE]

Photochemical and Radiation Sciences

Ames Laboratory
Ames, Iowa 50011

Division of Fundamental Interactions **$270,000**

7. ***Laser Spectroscopy and Electron Energy Transfer of Light Conversion Systems***
G.J. Small

This project centers on the structural organization and intermolecular interactions of pigments in artificial and naturally occurring photosynthetic aggregates and the utilization of efficient electronic energy transport in biomimetic chromophoric polymers in solar energy conversion. A variety of laser spectroscopies are utilized (e.g., optical hole burning, fluorescence line narrowing, picosecond spectroscopy). In addition, nonlinear laser spectroscopies are used to study coherent unidirectional energy transfer and the vibrational structure of molecular solids. [2.48 FTE]

8. ***Picosecond Spectroscopy and Reaction Dynamics***
W.S. Struve

This work concerns kinetic studies of organic redox photoreactions of species attached to semiconductor surfaces using picosecond fluorescence, absorption, and photocurrent transients. Measurements of excitation transport and trapping of dyes on surfaces and electron transfer from dyes into semiconductors are made using fluorescence spectroscopy. Mechanisms of vibrational energy transfer of large molecules in solution and gas phase are determined as well as photodissociation processes. [2.75 FTE]

Argonne National Laboratory
Argonne, Illinois 60439

Division of Chemistry **$4,134,000**

9. *Preparation of Organisms, Photosynthetic Pigments, and Biological Materials of Unusual Isotopic Composition*

H.L. Crespi, J.J. Katz, J.R. Norris, M. Wasielewski

This program has as its objective the production of photosynthetic microorganisms substituted with biologically important stable isotopes. The major effort is in the production of fully deuterated organisms, but in addition, the Argonne National Laboratory (ANL) Chemistry Division is able to grow organisms in which non-magnetic ^{12}C is replaced by magnetic ^{13}C, ^{14}N by ^{15}N, ^{16}O by ^{17}O or ^{18}O, and ^{24}Mg by ^{25}Mg. Large quantities of green algae, blue-green algae, and photosynthetic bacteria are routinely available in unnatural isotopic composition involving either single or multiple substitution. These organisms, and the compounds obtainable from them, have important applications in magnetic resonance spectroscopies, small-angle neutron scattering, and resonance Raman spectroscopy. Typical areas of interest are applications in the study of chlorophyll, photosynthesis, biomimetic photochemistry, and bacteriorhodopsin. Of particular importance is the ability to provide material for the growth of single crystals that contain unusual isotopes. [1.0 FTE]

10. *Gas-Phase Radiation Chemistry and Photochemistry*

C.D. Jonah, W.A. Mulac, A.D. Trifunac, D.B. McDonald, M.C. Sauer, Jr.

In this program, rate constants for simple free radical reactions are being measured, many of which are of great importance in atmospheric and combustion chemistry. The pulse radiolysis technique makes it possible to measure the kinetics at pressures of one atmosphere and above and over the temperature range of 50°C to 1000°C, a range no other single experimental technique can easily span. The reaction rates of OH and OD radicals with CO and simple organic compounds are under investigation. In addition to the practical importance of these reactions to combustion, the data serve as an excellent test for reaction theories because of the rigorous restrictions provided by the wide temperature range and the use of two hydrogen isotopes. [3.3 FTE]

11. *Chlorophyll and Photosynthesis Research*

J.J. Katz, J.C. Hindman

The principal objective of this research is to acquire sufficient knowledge about chlorophyll function in natural photosynthesis to make possible ultimately the replication of the natural primary light conversion event outside the living cell. Current research focuses on: (1) laser photochemistry and photophysics of chlorophyll and chlorophyll model systems; (2) new methods for the synthesis of chlorophyll and bacteriochlorophyll model systems; (3) characterization of a new chlorophyll from a recently discovered photosynthetic bacterium, *Heliobacterium chlorum*; (4) applications of californium-252 plasma desorption mass spectroscopy and high performance liquid chromatography to chlorophyll compounds and model systems; (5) structural studies by small angle neutron scattering of chlorophyll aggregates and natural photoreaction centers; and (6) possible homologies between bioluminescent bacteria and dinoflagelates and photosynthetic organisms. [3.6 FTE]

12. *Electron Transfer and Energy Conversion and Storage*

J.R. Miller, D. Meisel, K.H. Schmidt, M.C. Thurnauer, W. Mulac

This program is directed at the fundamental understanding of electron transfer between molecules held apart at fixed distances and the study of chemical mechanisms involved in the conversion and storage of light energy. Electron transfer rates are measured by pulse radiolysis of solids or compounds containing two functional groups separated by rigid molecular spacers to determine the effects of distance, energy, and molecular structure. The work on energy conversion and storage utilizes various microenvironments (1) to enhance charge separation and thus the efficiency of photoelectron transfer, and (2) to increase the yield of photo-redox products while minimizing the rates of back reactions. Particular attention is given to mechanistic studies of catalytic water-splitting in colloidal systems and in microenvironments such as micelles, polyelectrolytes, and membranes. [8.1 FTE]

13. *Physiochemical Investigations of Photosynthesis*

J. Norris, M. Wasielewski, M. Bowman

The goal of this research is to elucidate the molecular mechanisms whereby light energy is converted into chemical charge separation. Natural photoreaction centers are investigated in detail so that efficient model systems can be constructed. Emphasis is placed on the determination of the structural arrangement during the natural photosynthetic charge separation process for duplication in artifical photosynthesis. Time-domain spectroscopy is used to measure distances, orientations and dynamics within the molecular components which participate in the transfer of electrons. Electron transfer events that occur in the range of a few picoseconds and longer are probed by optical and magnetic techniques. Magnetic methods and theory are developed specifically to characterize picosecond charge separation in chemical systems. Charge separation in single crystals of the reaction centers of several photosynthetic bacteria is also a subject of investigation by means of magnetic and optical spectroscopy as well as x-ray and neutron diffraction. [5.1 FTE]

14. *Radiation Chemistry and Photochemistry in Condensed Phases*

A.D. Trifunac, C.D. Jonah, M.C. Sauer, Jr., S. Gordon, K.H. Schmidt

The objective of this program is the study of chemical and physical processes that follow ionization (or photoionization) in both polar and nonpolar liquids. This is relevant to radiation chemistry, for the understanding of breakdown in dielectric liquids, and for the understanding of charge separation, recombination, and transfer, phenomena which are the basis of chemical and biological processes of energy storage and utilization. Various methods of radiation chemistry and photochemistry are used to provide details of the nature and dynamics of the early transient species and their chemical fates. This includes the study of electrons and positive ions, radical ions and excited states, and the subsequent fragmentation of the excited species into radicals and molecular species. Spin dynamics in radicals and radical ions is being used to provide better understanding of reaction kinetics. Essential tools used in this program are the Argonne high-current picosecond electron linac, the pulsed Van de Graaff accelerator, and innovative, time-resolved, magnetic resonance and laser techniques which are being developed and applied to these problems. [15.3 FTE]

15. Artificial Photosynthesis
M. Wasielewski, J.R. Norris

The goal of artificial photosynthesis research is the development of molecular systems in the laboratory that not only mimic but improve upon natural photosynthetic energy conversion. This work focuses on several interrelated facets of this problem. First, a molecular design project involves the synthesis of molecular models of the natural energy conversion system. These models, through their mimicry of features of natural photosynthesis, aid in the structural and mechanistic understanding of the natural process. Second, the photophysics and photochemistry of these systems are studied with emphasis on light-induced electron transfer reactions. Advanced spectroscopic techniques such as picosecond spectroscopy and time-domain magnetic resonance are used to study these ultrafast processes. Third, the primary photosynthetic processes themselves are being investigated with a view toward integrating the information obtained from the laboratory systems with new knowledge of natural photosynthesis. [3.2 FTE]

Brookhaven National Laboratory
Upton, New York 11973

Dept. of Applied Sciences **$1,120,000**

16. Porphyrin Chemistry
J. Fajer

This program addresses the function of chlorophylls in the photosynthetic transduction of light into chemical energy, the catalytic role of porphyrins in bioenergetic enzymic reactions, and the application of these reactions to synthetic multi-electron photocatalysts for the fixation of carbon and nitrogen, and the decomposition of water. The work encompasses synthetic, structural, physical, and theoretical chemistry and presently includes: (1) the storage and transfer pathways of oxidizing equivalents in peroxidases and photosystem II; (2) the six-electron reduction of nitrite to ammonia mediated by isobacteriochlorins; (3) theoretical and experimental modeling of environmental effects (ligands, charges, Schiff bases, conformations) on the properties of porphyrin and chlorophyll radicals; and (4) x-ray and neutron studies of bacteriochlorins and chlorobium chlorophylls as models for exciton and electron migration, and self-assembled aggregates of these chlorophylls as models of the light harvesting antenna of green and brown photosynthetic bacteria. [6.6 FTE]

17. Electrochemistry and Photoelectrochemistry
S. Feldberg, T. Skotheim

The objective of this program is the understanding of a variety of electrochemical and photoelectrochemical phenomena. Areas of interest comprise both theory and experiment. Theoretical studies comprise (1) analysis of the effect of picosecond irradiations of semiconductor systems (elucidation of factors affecting bulk and surface electron-hole recombination), (2) analysis of the electrochemical switching of conducting polymers (faradaic and capacitive processes are shown to be inseparable–seemingly anomalous data obtained for chemical switching can now be shown to be consistent with electrochemical data), and (3) analysis of the underlying phenomena of diffusion and conductance in redox polymers (random walk and percolation analysis relate fundamental electron transfer kinetics to diffusion and/or conductivity). Experimental studies comprise (1) investigations of photoelectrochemical cells utilizing junctions between polypyrrole coated semiconductors and poly-(ethylene oxide) doped with KI/I_2, a solvent free solid polymer electrolyte, (2) investigations of the use of doped poly-(ethylene oxide) in electrochemical cells compatible with the ultra high vacuum required by spectroscopic techniques such as ESCA, SEXAFS, and NEXAFS, (3) investigations of modified polypyrrole films incorporating redox species (e.g., phthalocyanines, ferrocene) to catalyze various electron transfer processes such as O_2 reduction, and (4) investigation of the spectro-electrochemistry of polypyrrole to elucidate the mechanism of electrochemical switching. [3.2 FTE]

18. Chemical Properties and Reactions of Mono- and Dinuclear Ferrocene Derivatives
M. Hillman

This program is an investigation of the preparation and properties of metallocenes and related compounds that are expected to have application in the energy program, especially toward the splitting of water. Particularly, for the oxidation of water, ferrocene derivatives with potentials high enough to oxidize water under neutral or slightly acid conditions are required. Preparation of compounds with these properties are under way. For the reduction of water, the mechanics of the generation of hydrogen from [1.1]ferrocenophanes with strong acids is under study. Rates for hydrogen formation have been determined for three ferrocenophanes. These results indicate that the orientation of the protons on the iron atoms is a significant condition for the reaction. An understanding of this reaction will enable further modifications of the ferrocenophane so that hydrogen may be obtainable from weak acids, perhaps even water. [3.5 FTE]

Dept. of Chemistry **$2,790,000**

19. Radiation Chemistry
B.H.J. Bielski, R.A. Holroyd, H.A. Schwarz

This program uses pulse radiolysis and photolysis to study the behavior of transient chemical species. Principal areas of investigation are: (1) properties and reactions of electrons in dielectric fluids; (2) photoionization in dielectric fluids; (3) formation and reactions of transition metal ion complexes in unusual oxidation states; (4) the nature of transition metal ion-hydroperoxyl radical complexes; and (5) other reactions of the hydroperoxyl radical. The studies of electrons in dielectric fluids are of prime importance in understanding the basic processes of radiation chemistry, in the development of new detectors for high energy physics and for EXAFS measurements, and in controlling dielectric breakdown in transformers. The studies of transition metal complexes and hydroperoxyl radical reactions are important in developing and understanding certain homogeneous catalysis systems and methods of chemical storage of solar energy. [7.5 FTE]

20. *Photochemical Energy Conversion and Solution Kinetics*
N. Sutin, C. Creutz, T.L. Netzel

Transition metal complexes strongly absorb visible light and readily undergo electron-transfer reactions. They are excellent mediators of outer-sphere light-induced redox reactions, many of which effect net storage of the light energy and can also provide homogeneous catalytic routes for the thermal and photochemical formation of H_2 or the reduction of CO_2. This program covers fundamental studies of the reactions of both excited-state and ground-state complexes. Since efficient light conversion and storage require the diversion of a significant fraction of the electronically excited molecules into useful reactions which must be driven in competition with rapid physical deactivation processes (luminescence and radiationless decay) and chemical back-reactions, a major project objective is the quantitative study of these physical and chemical deactivation processes. In addition, because the overall efficiency of the conversion sequence may be limited by the nature and rate of the subsequent chemical steps, mechanistic studies of the reactions of transition metal ions in high and low oxidation states are being conducted. [10.4 FTE]

21. *Energy Transfer in Chemical Kinetics*
R.E. Weston, J.M. Preses

Chemical reaction rates depend strongly on the distribution of reactant energy among translational, rotational, vibrational, and electronic degrees of freedom. Conversely, the energy distribution in reaction products provides a sensitive probe of the reaction dynamics. Collisional energy transfer plays an important role in the reaction mechanism as a process by which energetic species are produced or removed. In this program, the transfer of translational, vibrational, or electronic energy is being studied. Atoms or molecules are produced in excited states by a pulse of ultraviolet, visible, or infrared radiation. The time-dependent disappearance of these excited species is monitored by the detection of radiation, either from the parent species or from molecules that have been excited by collisional energy transfer. This program also supports both in-house research and assistance to outside users at the Dynamic Spectroscopy Beamline on the VUV ring of the National Synchrotron Light Source. [5.7 FTE]

22. *Chemistry of Energetic and Transient Species in the Gas Phase and on Surfaces*
A.P. Wolf, R.A. Ferrieri

This program investigates the basic chemistry of atomic and molecular species in neutral or charged states possessing electronic and translational excitation. Included are studies of the reactive intermediates produced by nuclear processes in the gas-phase and of the reaction pathways available to C, N, O, and halogen atoms during atom-molecule encounters. New methods of atomic species generation will use synchrotron light to produce concentrations of molecular ions high enough to allow standard instrumental analysis of the final products. The Chemistry Department mass separator will be used to produce intense beams of charged ions and atoms of oxygen and nitrogen, for reaction with hydrocarbons and other compounds. A second effort of this program uses cyclotron-generated radionuclides in catalyst research, permitting studies to be performed at femtomolar concentrations. [5.7 FTE]

National Synchrotron Light Source	**$4,470,000**

23. *National Synchrotron Light Source Operations and Development*
M. Blume

The objective of this program is to support operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers: (1) operation and maintenance of the two NSLS electron storage rings and its associated injector combination of linear accelerator-booster synchrotron; (2) operation and maintenance of the photon beam lines of the VUV and X-ray storage rings; and (3) the technical support of experimental users. Development of the NSLS encompasses the further improvement of the storage rings by means of new developments in high resolution photon optics, state-of-the-art monochromators, X-ray mirror systems, detectors, and so forth. The NSLS storage rings will provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources. An extensive research and development program is necessary to optimize performance characteristics and to develop new beam line instrumentation that will permit users to take advantage of the unique research capabilities to be offered by this important new facility. This research and development effort also provides information which will support the construction of the beam lines and devices to be funded under the Phase II construction project. [49.5 FTE]

Lawrence Berkeley Laboratory
Berkeley, California 94720

Chemical Biodynamics Division	**$920,000**

24. *Artificial Photosynthesis*
M. Calvin, J.W. Otvos

We are seeking to devise a synthetic system to accomplish a photoinduced electron transfer across phase boundaries, the way natural chloroplasts convert light into chemical energy. We have demonstrated the transfer of electrons across the lipid walls of vesicles. Other types of charged, single surfaces such as SiO_2 colloid have been found to increase the reaction yield when a primary reaction product is electrostatistically prevented from back-reacting. We have shown that polymeric sulfonates can also produce this result. Presently, we focus on the catalysts which will be required at both the oxidation and reduction ends to produce the final products (e.g., hydrogen and oxygen). An iron-sulfur cluster has produced hydrogen electrochemically, but not yet photochemically. Certain cobalt complexes can be photochemically reduced to produce hydrogen. On the oxidation side, the natural catalyst is a manganese compound of unknown structure. We have shown that a manganese III porphyrin in a suitable microenvironment can be electrochemically oxidized to produce MnII and O_2. The next step is to perform the same reaction photochemically. [6.0 FTE]

25. *Picosecond Photochemistry*
J.H. Clark

Proton-transfer and electron-transfer reactions of electronically excited molecules form the basis for virtually all existing and proposed methods for the photochemical fixation of solar energy. In this research, the techniques of picosecond laser spectroscopy are used to directly monitor, in real time, the dynamics of these ultrafast processes. Such studies provide insight into the details of the mechanism and kinetics of these reactions at the molecular level. This work has shown that the naphthols, substituted naphthols, and substituted phenols provide prototypical systems in which the dynamics of excited-state proton-transfer are exquisitely sensitive to subtle chemical changes. The effects of solvent environment, intermolecular and intramolecular hydrogen bonding, molecular conformation, and reactant geometry are being studied with the aim of quantifying their role in excited-state proton-transfer processes. Picosecond time-resolved resonance Raman spectroscopy and time-resolved emission spectroscopy are being carried out on a number of electronically excited organometallic complexes to establish the changes in geometrical and electronic structures which occur upon photoexcitation. Picosecond dynamic photoselection spectroscopy has been developed and is being used to probe the symmetries of the excited electronic states of large molecules in solution. [2.7 FTE]

26. *Photon Conversion*

G.C. Pimentel, H. Frei

This research investigates the chemistry and energy movement as it occurs on electronically excited hypersurfaces. Since both natural and artificial photosynthetic processes depend upon the chemistry of electronically excited molecules, these studies aid in the design of systems for chemical storage of photon energy. Cryogenic solids furnish particularly favorable environments for the study of light-initiated and reaction-initiated movement between and on electronic hypersurfaces. Reactants under study include $O_2(^1\Delta_g)$, Hg ($^3P_1$ and $^1P_1$), and NH ($^1\Delta$ and X $^3\Sigma$) with various unsaturated compounds. The reaction between imidogen and dimethylacetylene provides various isomeric products and an interesting system for hypersurface mapping. Energy storage using near infrared light, photochromism, and hypersurface mapping are goals. Temporal aspects of electronically excited transient intermediates are examined using nanosecond infrared spectroscopy. [6.0 FTE]

Materials and Molecular Research Division — $470,000

27. *Photochemistry of Materials in the Stratosphere*

H.S. Johnston

This project is equally interested in fundamental physical-chemical studies of small molecules and in obtaining useful atmospheric data. Laboratory studies are carried out to obtain optical cross-sections, quantum yields, infrared line shapes and absolute intensities, pressure-broadening coefficients, information about microscopic states, and macroscopic rate coefficients for molecules and reactions currently important toward interpreting atmospheric observations. The experimental methods include visible and ultraviolet laser flash photolysis, laser resonance absorption, resonance fluorescence, and infrared diode lasers. Theoretical methods include some molecular quantum mechanics and some numerical atmospheric modeling. This research has applications to problems of atmospheric ozone, and recently it has become apparent that this field of research is applicable to the role of gases other than carbon dioxide on the "greenhouse effect." [4.6 FTE]

28. *Photon-Assisted Surface Reactions, Materials, and Mechanisms*

G.A. Somorjai

This project explores photocatalyzed chemical reactions that take place at the solid-liquid interface. These reactions include the photodissociation of water to produce hydrogen and oxygen and the photon-assisted reactions of carbon dioxide and water to produce simple hydrocarbons (photosynthesis). The purpose is to explore the mechanism of photon-assisted surface reactions and then to establish the optimum conditions (of surface structure, composition, temperature, and reactant mixture) to maximize the rate of production of the desired chemicals (hydrogen and/or hydrocarbons). The materials being used include iron oxides, silicates, and sulfides of rhenium and molybdenum. [3.0 FTE]

Notre Dame Radiation Laboratory
Notre Dame, Indiana 46556

$2,835,000

29. *Theoretical Studies On Reacting Systems*

D.M. Chipman, J.J. Kozak, W.M. Huo

Quantum and statistical mechanics methods are being developed to interpret phenomena in radiation chemistry and photochemistry, especially those involved in chemical-dynamic processes related to energy storage and transfer. A comprehensive statistical mechanical theory of photo- and radiation-induced redox reactions in organized molecular assemblies, such as monolayers and micelles, is being developed. These latter studies have considerable relevance to our understanding of experiments in which organizates may be applied in photochemical processes to effect the storage of solar energy. New quantum mechanical methods to perform and analyze electronic structure calculations on molecules and transient free radicals are being developed and used in conjunction with existing methods to study microscopic properties, such as molecular structures, potential energy surfaces, reaction mechanisms, photochemical properties, intermolecular forces, electron-solvent interactions, spin density distributions, and various spectroscopic parameters of molecules. Quantum dynamical aspects of the interaction of radiation with matter, specifically the temporal decay of excited states of two- and three-level atomic and molecular systems, are being studied using new analytical techniques. [11.0 FTE]

30. *Organic Photochemical Processes*

P.K. Das

Nanosecond laser flash photolysis experiments are being carried out to examine the role of intermediates (radicals, biradicals, singlet and triplet states, exciplexes, and ion pairs) on the photochemical reactions of organic systems in solution. Included are studies of addition, fragmentation, hydrogen abstraction and electron transfer reactions, intermolecular energy transfer between quasi-isoenergetic triplets, intramolecular transfer in molecules containing two chromophores, electron exchange interactions with stable radicals, energy hopping along a polymeric chain and energy trapping in copolymers containing several types of chromophores. Model systems being investigated include phenyl substituted polyenes and polyynes containing heteroatoms, aromatic hydrocarbons and carbonyl compounds, small ring heterocyclic systems, stilbene analogues and polymers containing carbonyl groups. The studies on energy migration in polymers are particularly relevant to photosynthesis and to possibilities for enhancing the properties of polymers toward photodegradation or photostabilization. Programmatic emphasis is on obtaining mechanistic details of photochemically induced reactions. [8.0 FTE]

31. *Inorganic Photochemical Studies*
G. Ferraudi

The photochemical properties of coordination complexes of the first and second row transition metal ions with macrocyclic and olefinic ligands are being investigated. Conventional laser flash photolysis methods are used and supplemented by product analysis. A sequential biphotonic excitation technique is also being used for probing the time and energy relationships between long-lived excited states. This research is carried out with compounds that exhibit either a direct or sensitized photochemical redox reactivity for excitation in the visible region of the spectrum and are, therefore, candidates for use in solar energy conversion. Two families of compounds are the main targets of these studies: complexes with macrocyclic ligands, namely phthalocyanines and more simple macryocycles, and metallocenes. Elucidation of general relationships between photoreactivity and the molecular structure of the macrocycles and the study of mechanisms which exhibit potential application as photocatalytic systems are essential goals of this project. [8.5 FTE]

32. *Microwave Studies On Radiation Chemically Produced Intermediates*
R.W. Fessenden

Electron spin resonance (ESR) spectroscopy is being used to study radical structures, radical reaction mechanisms and kinetics, and the nature of electron spin interactions in fluids. Continuous *in situ* radiolysis generates radicals for characterization of their geometric and electronic structures by means of the observed ESR hyperfine patterns. The identity of the radicals produced and any subsequent transformations observed provide information on reaction mechanisms. Time-resolved experiments on radicals produced by pulse radiolysis measure reaction rates for intramolecular rearrangements and bimolecular disappearance, as well as rates of bimolecular spin relaxation and the extent of signal enhancement by chemically induced dynamic electron spin polarization. The latter quantities, taken together with reaction rates, provide very detailed information on reaction mechanisms in liquids. Pulsed microwave experiments, including the use of saturation recovery and electron spin echo techniques, provide information on relaxation times in a more direct way. The spin echo method also allows improved time resolution for fast reaction rate measurements. Microwave methods are also used to study electron attachment processes in high pressure gases and liquids. [6.5 FTE]

33. *Time-Resolved Studies of Photolytic Reactions*
R.W. Fessenden

Time-resolved microwave absorption methods are applied to characterize the charge distribution in intermediates produced by laser excitation. Particular attention is being given to measuring the dipole moments (i.e., the degree of charge separation) in various radicals, excited states, and exciplexes that are intermediates in photochemical processes. Parallel optical experiments employing two lasers, one to form and the second to photolyse the intermediate states, are also being carried out. Applications are directed toward characterizing the various absorption bands of the intermediates in terms of their photochemical activity. Optical absorption spectroscopy is used for diagnosis. Where dissociation is observed, studies of the recombination kinetics of the resultant fragments often provide rate data not directly available. Two-pulse experiments involving laser photolysis and pulse radiolysis are also used to investigate photochemical activity of radiation chemical intermediates and reactivity of photoexcited states with radicals. These investigations are complimented by both steady-state and time-resolved ESR studies of photolytically produced radicals. [5.5 FTE]

34. *Theoretical Aspects of Radiation Chemistry*
K. Funabashi, A. Mozumder

These studies relate to the physical and chemical behavior of the electron in its various aspects and in different phases. Attention is focused on the development of a unified theoretical framework capable of describing the various physico-chemical properties of solvated electrons such as their optical absorption spectra and transport properties. Problems associated with thermalization of radiation produced electrons in both gases and liquids are addressed to elucidate the nature and properties of reactions at early times, especially as they apply to track effects. Contributions of secondary electrons to the reactions within heavy particle tracks are being examined. The thermalization studies are being extended to examination of the time evolution of the effective electron temperature in molecular gases based on experimentally available elastic and inelastic cross-sections. Conclusions from these various studies are important both to many aspects of radiation chemistry and to applications where ions are important in, for example, fluorescence detectors and solid-state devices. [3.0 FTE]

35. *Spectroscopy of Reaction Intermediates*
J. Hardwick

Laser-excited fluorescence, chemiluminescence, and laser intracavity absorption spectroscopy are being used to carry out high resolution spectroscopic studies of small molecules, free radicals, and molecular ions in the gas phase. These spectra yield information essential for the accurate monitoring and identification of some of the highly reactive species found in flames, as well as aiding in the prediction of their reactivity based on energetic and symmetry considerations. High-lying vibrational levels of molecules ranging in size from diatomic to small aromatic molecules are being studied at rotational resolution in their ground and excited electronic states through their optical spectra. Collisional transfer of rotational, vibrational, and electronic energy is being investigated in small molecules to aid in the development of qualitative and quantitative descriptions of the pathways by which electronic energy is thermalized in such diverse systems as flames, electric discharges, and gas lasers. [2.0 FTE]

36. *Photochemical Processes Following Core Electron Excitation*
R.G. Hayes

Photochemical processes which follow excitation of 1s electrons in molecules containing several different first-row elements are being examined to determine the dependence of the photochemical processes on the specific atom which is excited. Initial efforts involve an examination of ionic photofragmentation processes in molecules such as formamide ($HCONH_2$) in which three distinct sites can be excited selectively. The experimental work is being carried out at the National Synchrotron Light Source using photons in the 200-500 eV region. The pathways of fragmentation are determined by the ionic electronic states left behind when the 1s holes decay by Auger processes. The distribution of these states depends on the atom which is excited initially. Thus, computational work on the valence Auger spectra of molecules, using the MS-Xα technique, is being carried out as well. [1.5 FTE]

37. *Influence of Ordered Molecular Assemblies On Chemical Processes*
L.K. Patterson

These studies are directed toward developing a better understanding of the relationships between structure in organized molecular assemblies and the influence these assemblies may exert on kinetic behavior in bulk phase, assembly pseudophase, or at interfacial boundaries. A variety of unique properties has been observed for systems in which such assemblies–micelles, vesicles, spread monolayers and liquid crystals–are formed. Such properties under study include compartmentalization of reaction into microregions with well defined boundaries, nonhomogeneous distribution of reactants, surface orientation of reactant molecules, surface charge effects, and reduction in dimensionality of the reactant phase. Alterations in rates and reaction mechanisms that are observed in such assemblies strongly suggest the possibility for kinetic control over a variety of photochemical and radiation chemical processes not possible in homogeneous solution. Principal attention is now directed toward studies in spread monolayers because these latter assemblies provide for significant control in the degree of organization which may be imposed on a reaction system. Investigations are being carried out also on photophysical behavior in liquid crystals which exhibit phases of varying organization. [8.0 FTE]

38. *Radiation Chemistry Data Center*
A.B. Ross, W.P. Helman, G. Hug, I. Carmichael

The Radiation Chemistry Data Center (RCDC) maintains and continuously updates a bibliographic data base on radiation chemistry and photochemistry and provides a variety of information services to the scientific community. Retrospective searches are carried out and bibliographies on specific topics are prepared and made widely available. A current-awareness publication, *Biweekly List of Papers on Radiation Chemistry and Photochemistry*, is produced from the data base and distributed to subscribers. Experimental data for reaction intermediates produced by light or ionizing radiation are compiled from the published literature. Data are included for photochemical and photophysical processes in solution. The data are stored in computer-readable files and are readily available for correlation and reformatting in various ways. Critical reviews of these data are prepared for publication. A goal of this program is the development of a numeric data base of kinetic and spectroscopic properties of reaction intermediates which can be effectively used by many types of users. These bibliographic and numeric data bases are expected to be of increasing importance in the basic scientific study of chemical processes in irradiated systems and in technological applications such as solar energy utilization and photochemical effects on the environment. [2.0 FTE]

39. *Radiation Induced Reactions*
R.H. Schuler, L.K. Patterson, G.N.R. Tripathi

A wide variety of chemical reactions induced by the absorption of ionizing radiation are being examined using the Laboratory's broad base of highly developed chemical and instrumental methods for examining intermediates, both in time resolved studies and by analysis of ultimate products. Improvements in dosimetry and time resolution at the LINAC pulse radiolysis facility allow detailed optical and conductometric pulse radiolytic studies to be carried out at nsec and longer times. Recent introduction of laser resonance Raman techniques allows parallel studies of time resolved vibrational spectra of intermediates. Currently, focus is on the molecular and electronic structure of oxygenated radicals present in electron transport processes. Radiation chemical studies are also being carried out at the Notre Dame Heavy Ion Facility to examine track effects in radiation chemical reactions induced by low Z ions having LETs of 1-100 eV/Angstrom. Studies are also being carried out at very high pulse intensities to examine the products of second order reactions between radicals using a Febetron as a radiation source. [21.0 FTE]

Solar Energy Research Institute
Golden, Colorado 80401

Solar Fuels Research Division **$625,000**

40. *Photophysics and Photochemistry of Porphyrins and Model Systems For Artificial Photosynthesis*
J.S. Connolly

This project is concerned with fundamental studies of energy- and electron-transfer processes of excited states in a variety of porphyrin-related systems. The focus is on detailed photophysical properties of porphyrins and on light-induced electron transfer in synthetic models of photoreaction centers. The goal is to contribute to an improved understanding of the molecular properties required for efficient light-induced electron transfer in artificial photosynthesis. Laser flash photolysis, fluorescence, and spectroscopic studies are being carried out on covalently linked porphyrin-quinones and on their unlinked constituents to sort out the effects of photophysical properties, redox potentials, molecular geometry, temperature and solvent properties (dielectric constant, viscosity) on the kinetics and mechanisms of light-induced electron transfer and subsequent charge stabilization. [0.8 FTE]

41. *Modified Semiconductor Electrodes For Solar Energy Utilization*
A.J. Frank

This research program addresses the fundamental problems of the photoinstability of n-type semiconductors and the high overpotential associated with specific chemical reactions such as the reduction and oxidation of water. Interfacial chemistry, energetics and surface dynamics are established by (photo)electrochemical measurements, end-product analyses, and surface characterization studies. Information obtained from the physicochemical investigations provides guidance for chemically modifying the semiconductor surface to improve photostability and kinetics of desirable redox reactions. The utility of coating the semiconductor surface with electrically conductive polymers in combination with catalytic dispersions of several transition metals is demonstrated for the visible light-induced water-cleavage reaction. Further development and study of conductive polymers and catalytic surface structures involving coordination metal complexes are in progress. The degree of stability and catalytic activity produced is remarkable and provides encouragement for the potential application of catalytic conductive polymer films to practical photoelectrochemical devices for solar energy conversion. [1.0 FTE]

42. Basic Photoelectrochemistry Research
A.J. Nozik, J.A. Turner

Basic research in photoelectrochemistry is being conducted in the following three areas: (1) hot carrier effects; (2) energetics, kinetics, and characterization studies of semiconductor-electrolyte interfaces; and (3) photoelectrochemical properties of colloidal and particulate semiconductors. Studies of hot electron injection processes from semiconductors into electrolytes are being extended to redox couples lying within the semiconductor band gap. Hot electron reduction of H^+ to H_2 on p-InP is being modeled, and theoretical current-voltage characteristics are being compared to experimental results. The relationship of hot carrier processes to catalytic processes is being analyzed, as well as the theoretical conversion efficiency of Type I hot carrier injection. Computer controlled techniques of photocapacitance, photocurrent and photovoltage spectroscopy, and Mott Schottky analysis are being developed. The techniques of pulse radiolysis and Moessbauer spectroscopy are being used to characterize the photoelectrochemical properties of semiconductor colloids and particles. The flat-band potentials and charge transfer kinetics of several semiconductor colloids and powders have been measured as a function of particle size. Size quantization and hot carrier effects in very small sized (<50 Angstrom) semiconductor colloids are being investigated theoretically and experimentally. [2.8 FTE]

Chemical Physics

Ames Laboratory
Ames, Iowa 50011

Division of Fundamental Interactions **$640,000**

43. Statistical Mechanics of Non-Equilibrium Systems
D.K. Hoffman

Statistical mechanics is used to develop kinetic theory of polyatomic gases in which transport, relaxation, and reactive processes are of interest. Classical and quantum mechanical scattering theory is utilized in the development of collision models to describe energy transfer and reaction between molecules with internal structure. The dynamics and statistics of distributions of molecules adsorbed on surfaces under non-equilibrium conditions is analyzed via master equations. Such a theory is important for the appropriate interpretation of surface spectroscopic data associated with these processes. This project includes an investigation of the effect of surface coverage on the nature of binding sites, an exploration of interactions between adsorbed surface species, a study of surface migration and cluster formation, and adsorbate effects on the catalytic properties of surfaces. These models for irreversible lattice processes are also applied to other (non-surface) systems. [1.95 FTE]

44. Atomic, Molecular, and Free Radicals: Crossed Beam Kinetics
C.Y. Ng

This project involves crossed molecular beam studies bearing on the kinetics of fundamental processes in combustion and low pressure pyrolysis of hydrocarbons. It also includes the molecular dynamics of excited atoms and molecules, ion/molecule reactions, and high resolution photoionization of molecules, clusters, and transient radicals. A coaxial reactor is being developed for photoionization sampling of reactions involving oxygen atoms and simple hydrocarbons. An important aspect of the work is to understand the role played by stable molecules, intermediate radicals, and ions in flames. [3.43 FTE]

45. Molecular Theory Bonding
K. Ruedenberg

Molecular properties, geometric electromagnetic and spectral, and in particular, energy changes during chemical reactions are determined through quantum chemical calculations of molecular electronic structures. Reaction energies and activation energies for elusive intermediates and transition states are predicted. Electronic rearrangements along reaction paths and their energetic and kinetic implications are analyzed. Fundamental developments in many-electron quantum mechanics including electron correlation are made, with the aim of achieving chemical accuracy by practical methods for predictions of reaction mechanisms. Quantitative interpretative concepts are developed for use by non-theorists to analyze reliably and anticipate intuitively *ab initio* predictions. Oxidation-reduction and exchange reactions involving carbon, nitrogen, oxygen, hydrogen, and silicon are studied, in particular reactions occurring in combustion, in the atmosphere, and during hydrogenations. [2.76 FTE]

46. Ion Chemistry–Mass Spectrometry
H.J. Svec, G.D. Flesch

This research involves the ion chemistry of inorganic, organometallic and organic compounds and ions and complementary neutral fragments produced by electron bombardment. The latter leads directly into the chemistry of highly excited molecules and free radicals. The results bear directly on the origin of aromatic heterocyclic hydrocarbons produced in the combustion of natural gas, oil, wood, and coal under fuel rich conditions. [1.45 FTE]

Argonne National Laboratory
Argonne, Illinois 60439

Division of Chemistry **$1,770,000**

47. Theoretical and Computational Chemistry
T.H. Dunning, Jr., R.A. Bair, M.J. Davis, L.B. Harding, R.L. Shepard

This program concentrates on theoretical studies of the energetics and kinetics of chemical reactions, with an emphasis on reactions of importance in the oxidation of hydrogen and simple hydrocarbon fuels. The basic thrust of the project is on calculation of accurate molecular interaction potentials, study of the chemical dynamics on the computed (or other realistic) potential energy surfaces, and characterization of the molecular species (including ephemeral species) involved. In addition, in FY 84 an exploratory program was initiated which will concentrate on theoretical studies of small clusters of transition metal atoms. The basic thrust of this program will be on the characterization of the electronic structure of the clusters. Finally, there is a continuing effort devoted to development of the theoretical and computational methodology needed to provide a realistic description of these fundamental chemical processes. [7.2 FTE]

48. *High Resolution Spectroscopy and Excited-State Dynamic Processes*

J.P. Hessler, F.S. Tomkins

The goal of this program is to elucidate the complex chemical processes needed to describe the behavior of polyatomic molecules which have been excited with vacuum-ultraviolet light. At this relatively high excitation energy the processes of autoionization, predissociation, direct molecular fragmentation, and the decomposition of "superexcited" states are important. High-resolution ($\delta E/E \sim 10^{6}$) excitation sources are used to selectively excite specific predissociative and Rydberg states of polyatomic systems which have been cooled by the supersonic free-jet expansion technique. A unique feature of this program is the development and utilization of a picosecond laser source which operates in the energy region between 5 and 11.3 eV (250 to 110 nm). With this source the development of the system is followed with 10-picosecond time resolution. The triatomic systems being studied include CO_2, H_2O, and XCN (X = H, D, I, Br, and Cl). [2.9 FTE]

49. *Molecular Beam and Metal Cluster Chemistry Research*

S.J. Riley, E.K. Parks, K. Liu

The study of heterogeneous catalysis on a molecular level is pursued. Beams of catalytically active naked metal (Ni, Cr, V, Ag, Cu, Al, Fe) atom clusters containing 2 to 200 atoms are generated by pulsed lasers, and their physical and chemical properties are characterized by laser based, in-flight diagnostic techniques. Spectral and electronic properties are determined and experimental results are correlated with theoretical calculations. Mechanisms and kinetics of cluster chemical reactions and of adsorption and catalytic processes on cluster surfaces are determined by the flow tube technique. The transient products are identified by laser ionization mass spectrometry. [5.6 FTE]

Brookhaven National Laboratory
Upton, New York 11973

Dept. of Applied Sciences **$583,000**

50. *Kinetics and Mechanisms of Alternative Fuels Combustion*

R.B. Klemm, J.V. Michael, J.W. Sutherland

The aims of this project are (1) to measure absolute rate constants for elementary combustion related reactions over a wide temperature range, and (2) to investigate mechanistic factors involved in gas phase combustion and pollutant formation processes. Emphasis is on alternative fuels that comprise a range of fuel types, including alcohols and hydrocarbon synfuels. In pursuing the goals of this project, a facility has been developed that features a variety of experimental techniques including: (1) flash photolysis-resonance fluorescence (FP-RF); (2) discharge flow-resonance fluorescence (DF-RF); (3) flash photolysis-shock tube-atomic absorption (FP-ST-AA); and (4) discharge flow-photoionization mass spectrometry (DF-PIMS). The FP-RF and DF-RF methods are used in determining specific rates of elementary atom-molecule and radical-molecule reactions over a wide temperature span, ~200-1100K. The recently developed flash photolysis-shock tube apparatus extends the high temperature capabilities for direct rate measurements by a significant extent. With this device, kinetic studies are performed over a temperature range from about 800K to about 2200K; and thus these measurements overlap the temperature range of the other, more conventional techniques utilized in this project. The DF-PIMS method is used in this project in an effort to make direct observations of reactants and products for elementary reactions to investigate the relevant reaction mechanisms. This DF-PIMS experiment utilizes the National Synchrotron Light Source (NSLS). [6.0 FTE]

Dept. of Chemistry **$2,668,000**

51. *Theoretical Chemistry*

S. Ehrenson, J.T. Muckerman, M.D. Newton

The goals of this project are to apply theoretical methods to the study of energy flow in chemical reactions and to the elucidation of molecular interactions involved in the storage and interconversion of energy in the gas phase and in condensed phases, including phenomena associated with charged species (i.e., solvation and charge-transfer processes). The methods principally used are *ab initio* and semiempirical calculations of the energies and structures of molecules in specific electronic states, and classical and semiclassical treatments of the nuclear motion in kinetic processes involving these systems. Many of the techniques currently being developed and applied in this project play an important role in analyzing and interpreting the data obtained in experimental projects in the Department. [7.1 FTE]

52. *Ion-Molecule Reactions With Applications to Fusion Energy Systems*

L. Friedman, R.J. Beuhler

The development of high molecular weight mass spectrometric techniques has provided a facility for the investigation of nucleation processes responsible for the formation of cluster ions and neutral microclusters. Immediate goals are the development of cluster-ion sources and their exploitation as a basic research tool. A high molecular weight mass spectrometer that has the capability of mass analysis of molecular species with m/e values up to approximately 200,000 is now in use. Efforts to expand this mass range to higher m/e values are pursued, using high voltage ion post-acceleration, and development of time-of-flight mass analytical techniques. Ion source facilities capable of generation of plasmas from gases cooled to temperatures as low as 10 K will be used to study cluster ion generation from inert gases and diatomic molecular species. The generation of cluster ions from hydrogen isotopes is considered a major project objective because of the potential role these cluster-ions may have in the study of controlled thermonuclear reactions. Use of clusters, accelerated to high kinetic energy, to imprint structure on solid surfaces with the generation of microscopic cavities or holes in thin films has been investigated as an additional, technically important application of cluster ion beams. [6.7 FTE]

53. *Gas-Phase Photoionization and Photoelectron Spectroscopy of Molecules and Clusters*

J.R. Grover, M. White

Fundamental data necessary to understand fast, exothermic gas phase reactions are being measured via photoionization of molecular beams. This work utilizes tunable, monochromatic radiation from the gas-phase beamline on the VUV storage ring at the NSLS. Excitation function measurements on mass-selected ions are being carried out for van der Waals and hydrogen-bonded dimers and clusters, free radicals, and molecules. From these data, heats of formation and binding energies are determined for both neutral and ionized species, especially neutral dimers, and studies are made of the Rydberg structure and dissociative ionization pathways of molecules and weakly-bound dimers from which an inner-valence electron has been excited or ejected. A general photoelectron spectroscopy study of the ionization dynamics of neutral molecular excited states utilizing both synchrotron and laser radiation is also under way. Photoelectron energy spectra are taken following VUV single-photon excitation or resonant, multiphoton ionization via excited vibronic levels above and below the ionization threshold, respectively. From the observed electronic and vibrational state distribution of the ion, it is possible to investigate in detail the electronic structure and ionization dynamics of electronically excited states of neutral molecules. [4.2 FTE]

54. *Structure and Bonding of Solids and Molecules On Their Surfaces*
J. Hrbek, T.K. Sham

The main objective of this research program is to improve the understand of (1) the electronic interactions between surfaces and adsorbates, and (2) the interactions among atoms in condensed matter, with emphasis on technologiclly important materials. Identification of molecular structure of surface intermediates, active sites on surfaces, and the effect of promoters and poisons on surface selectivity and activity will help to understand and control the chemistry of surfaces. These studies are being carried out through photoelectron spectroscopy, thermal desorption, electron diffraction, vibrational spectroscopy, and the development and application of synchrotron radiation spectroscopies, such as photoelectron and x-ray absorption (XANES and EXAFS). The results of these studies are directly related to kinetic and mechanistic aspects of chemical reactivity and catalysis. [3.5 FTE]

55. *Chemical Crystallography*
T.F. Koetzle, A. Kvick, R.K. McMullan

Neutron and x-ray diffraction methods are used to solve significant problems in crystal and molecular structure. Emphasis is placed on structures where hydrogen and other light atoms are important and on disordered or partially-ordered structures, since in these areas neutron diffraction, alone or in combination with x-ray diffraction, has unique advantages for determining molecular structure and investigating chemical bonding. Completion of the chemical crystallography beamline at the National Synchrotron Light Source will open up new areas for x-ray diffraction studies. Examples of systems investigated under the crystallography program include organometallic compounds, transition-metal hydrides, zeolites, fast-ion conductors, and dielectric materials. [4.6 FTE]

56. *Spectroscopy and Structure of Short-Lived Chemical Intermediates*
T. Sears

Studies of the structure and reactivity of molecular fragments are important in our understanding of gas phase chemical reaction pathways and rates. Infrared laser techniques are to be applied to the study of these species, which are usually unstable and present only in trace quantities in reaction mixtures. Analysis of the spectra will lead to details of molecular structure, intra- and inter-molecular potential functions, and estimates of the concentrations of reaction intermediates involved in the course of reactions important in combustion and in semiconductor technology. [1.5 FTE]

Lawrence Berkeley Laboratory
Berkeley, California 94720

Applied Science Division **$125,000**

57. *Unimolecular Kinetics*
N. Brown

Combustion chemistry consists of complex, chain mechanisms involving radical species. The inherent difficulties encountered in high temperature environments, and the large number of species involved in hydrocarbon oxidation make the study of combustion chemistry difficult. One activity of the current research is concerned with the application of theoretical chemical kinetics to study high temperature kinetics important in combustion. Emphasis has been placed upon investigating the dynamics of reactions using classical trajectories. Unimolecular and bimolecular reactions are investigated with realistic potential energy surfaces. Special emphasis has been placed upon elucidating the role of molecular angular momentum of intramolecular and intermolecular energy transfer processes. Rate coefficients for reactions important in combustion are also determined with statistical theories. A second activity is concerned with investigating the ignition chemistry of hydrocarbon/air mixtures. Identification of the principal elementary reaction steps which occur during ignition of hydrocarbon/air mixtures and determination of the corresponding rate coefficients are required to achieve an understanding of ignition. Initially, ignition will be investigated in a static system and the time-resolved evolution and decay of active radical species will be monitored. Temporal measurements of radical concentrations will be achieved with a molecular beam mass spectrometer and with spectroscopy. [1.25 FTE]

Materials and Molecular Research Division **$2,326,000**

58. *Energy Transfer and Structural Studies of Molecules on Surfaces*
C.B. Harris

A proper description of the ways in which internal energy is transferred between molecules and surfaces through electromagnetic field interactions, particularly in the short distance regime, is crucial to the understanding of a wide variety of molecule-surface interactions including laser induced photoionization and photochemistry at metal and semiconductor surfaces. In addition, surface enhanced electromagnetic field interactions are fundamental to other phenomena such as surface Raman scattering and other non-linear interactions. The long-range goals of this research are (1) to study and understand the general principles that underlie electronic and vibrational energy redistribution at metal surfaces, and (2) to develop new laser techniques for characterizing metal surfaces and chemisorbed molecules in the visible and vibrational infrared portion of the electromagnetic spectrum. [2.2 FTE]

59. Crossed Molecular Beams
Y.T. Lee

The major thrust of this research project is to elucidate detailed dynamics of simple elementary reactions which are theoretically important and to use the molecular beams method to unravel the mechanisms of complex chemical reactions or photochemical processes which play an important role in many macroscopic processes. Molecular beams of reactants are used to study individual encounters between molecules or to monitor photodissociation events in a collision-free environment. Most of the information is derived from measurement of the product fragment energy and angular distributions using a unique molecular beam apparatus designed for these purposes. Recent activities are centered on the direct probing of transition states of the $F + H_2$ reaction through the experimental observation of quantum mechanical resonance phenomena, the mechanisms of elementary chemical reactions involving oxygen atoms with unsaturated hydrocarbons, the dynamics of chemical reactions of electrochemically excited atoms, the primary photochemical processes of polyatomic molecules radicals and ions, intramolecular energy transfer of chemically activated and locally excited molecules using overtone excitation processes, and the interaction potential of open shell atoms with rare gas atoms. [8.0 FTE]

60. Molecular Interactions
W.A. Lester, Jr.

This program is directed at extending fundamental knowledge of the interactions that govern the dynamics of energy transfer, reactive, and photodissociative molecular processes. The approach is based on the reliable description of the potential energy surfaces and coupling matrix elements needed in theoretical approaches for the evaluation of cross sections and rates. Emphasis is placed on the use of state-of-the-art Hartree-Fock (HF), multiconfiguration HF, and configuration interaction (CI) *ab initio* methods for the accurate description of molecular interactions. A variety of methods are used to describe collision dynamics. The electronic structure studies emphasize the determination of the critical geometries and energetics that govern reaction pathways and include the computation of global potential energy surfaces where appropriate. The dynamics studies include fully quantum mechanical approaches to ro-vibrational energy transfer in molecules by collision, and an adiabatic approach to single-photon photodissociation of small polyatomic molecules and to chemical reaction. A novel method that solves the Schroedinger equation stochastically is also being studied to ascertain its usefulness for determining the energy and other molecular properties. [3.5 FTE]

61. Theory of Atomic and Molecular Collision Processes
W.H. Miller

This research is primarily involved with the development of theoretical methods and models for describing atomic and molecular collision processes. Specific topics of interest include the theory of inelastic and reactive scattering, collision processes involving electronically excited atoms or molecules, collisional ionization phenomena, statistical theories of chemical reactions, scattering of atoms and molecules from surfaces, and the interactions of molecular systems with high power laser radiation. Much of this research is involved with the development and application of a general semiclassical mechanics that allows one to combine classical mechanics and quantum mechanics in a correct and useful manner. This has been extremely successful in providing an understanding of the various quantum effects that are seen in molecular phenomena, and it also often provides simpler computational methods for carrying out quantitative calculations. Certain research topics are more amenable to a completely quantum mechanical approach, and these sorts of theoretical techniques are also used. The ability to understand–and thus to model and to predict–chemical kinetics phenomena in the gas phase has widespread practical importance in a number of different areas. Among these are atmospheric chemistry and physics, interactions of molecules with strong laser fields, and energy transfer and chemical reactions in flames and combustion. [3.8 FTE]

62. Selective Photochemistry
C.B. Moore

The goals of this program are to understand the photophysics of selective excitation of molecules, dynamics of energy transfer and specificity loss, and the chemical reactions of specifically excited states. Low levels of vibrational excitation in small molecules, chemical reaction rate constants are defined for each quantum state. Larger, more highly excited molecules, energy is usually transferred among vibrational modes more rapidly than chemical reactions occur. The nature of the energy states of molecules as a function of excitation energy and of molecular size and structure determines the intramolecular flow of energy. The possibilities for limitations upon selectivity in photochemical processes are determined by the time evolution of the combination of spectroscopic states excited by the photons. A complete understanding of unimolecular dynamics is sought by both the examination of spectra and the measurement of reaction rates. Rates and mechanisms of free radical reactions are often best studied by flash kinetic spectroscopy using laser, for thermal heating, for photolyzing, and for spectroscopic probing. A fundamental understanding of these reactions is ought to serve as a basis for modeling combustion processes. Radical-radical collisions can lead to complex formation. Consequently, reactions and energy tranfers between radicals can be understood in terms of unimolecular reactions. [3.0 FTE]

63. Physical Chemistry With Emphasis On Thermodynamic Properties
K.S. Pitzer

The purpose of this program is the discovery and development of methods of calculation of thermodynamic and related properties of important chemical systems by use of quantum and statistical mechanics together with experimental measurements for key systems. Primary emphasis will be on ionized systems, electrolyte solutions, and plasmas. Systems comprising fused salts mixed in any proportion with water are being studied experimentally and with semiempirical theory. Recent theoretical advances include treatments of the dielectric constant of H_2O, the thermodynamics of ionic solutions in H_2O above its critical temperature, and the critical properties of pure ionic fluids such as NaCl. Earlier advances yielded improved equations for electrolyte solutions which are now being applied to a wide variety of systems of industrial or geological interest including geothermal brines. Current efforts also include relativistic quantum mechanical methods for the calculation of energies, bond distances, and other properties of the ground and excited states of molecules containing very heavy atoms where the conventional nonrelativistic methods are inadequate. Such results are important in evaluation of possible laser systems and for models of catalytic entities including heavy atoms such as platinum. [2.2 FTE]

64. *Spectroscopy and Structures of Reactive Intermediates*
R.J. Saykally

The principal objective of this program is to study spectra, structures, and properties of elusive reaction intermediates that are of importance in combustion processes. Present emphasis is on the development of three powerful new spectroscopic techniques for detecting very low concentrations of such reactive intermediates. A far-infrared laser magnetic resonance (LMR) spectrometer employing selective UV photolytic generation of the reactive species is presently being tested; optimization of the experimental parameters for study of the hydroxyl radical has been accomplished. Extension of this approach for the study of important carbene species (HCOH, HCCN, CH_2) is in progress. A totally new laser spectroscopy experiment has been developed. Molecular Beam Laser Electronic Resonance (MBLER), in which ultra cold (10-50°K) reactive molecules are generated in supersonic beam inside the cavity of a far-infrared laser and rotational transitions are tuned into resonance with the laser with a large DC electric field, compliments the capabilities of Laser Magnetic Resonance for the study of reaction intermediates. The system is being tested on stable molecules (CH_3F, PH_3) and will be extended to prototype reactive intermediates (OH, CH, CH_2) in the near future. The first measurement of the dipole moment of methylene (CH_2) is anticipated. [3.7 FTE]

65. *Potential Energy Surfaces For Chemical Reactions*
H.F. Schaefer, III

This research program has two goals, related yet distinct. The first goal is the development of new theoretical and/or computational methods for the description of "what electrons are doing in molecules," to use the words of Robert S. Mulliken. Specifically, the single outstanding problem in the field is the correlation problem, that of formulating models for going beyond the single-particle or Hartree-Fock approximation. The second goal of research is to apply these theoretical methods to significant problems of broad chemical interest. Currently, two areas are of special interest: (1) model theoretical studies of chemisorption, metal clusters, and organometallic species; and (2) potential energy surfaces which govern gas-phase chemical reactions. Research in the former area is ultimately aimed at a truly molecular understanding of catalysis, a subject pertinent to future energy requirements but sometimes approached by trial and error methods. In the latter area, research sometimes tends toward molecules potentially important in combustion or atmospheric chemistry and the development of high power laser systems. It is to be emphasized that in recent years theoretical chemistry has become a significant source not only of broad generalities, but also of specific predictions concerning molecular systems which may be very important but inaccessible to experiment. [5.5 FTE]

66. *Photoelectron Spectroscopy*
D.A. Shirley

This program addresses experimental aspects of electron spectroscopy to investigate the electronic structure of matter. General areas under study include: (1) electron spectroscopy, electronic structure of matter, as determined by photoelectron spectroscopy and related techniques; (2) the electronic structure of gas-phase species, including high-temperature species, as determined by the use of pulsed synchrotron radiation, including absorption and time-of-flight photoelectron spectroscopy; (3) photoelectron angular distributions and correlation-state studies; (4) electronic structure of solids from angle-resolved, variable-energy photoemission; (5) atomic and electronic structure of surface-adsorbate systems; (6) photoelectron spectroscopy of metal clusters and other exotic species; and (7) exploration and development of new experimental methods based on synchrotron radiation in the energy range 10-4000 eV, such as photoelectron diffraction, ARPEFS, and surface EXAFS. [10.5 FTE]

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Chemistry Division	**$438,000**

67. *Molecular Research With Electron Spectroscopy*
T.A. Carlson, M.O. Krause

A basic study of the photoelectron dynamics of molecules and metal vapors is being undertaken through the use of angle-resolved photoelectron spectroscopy and synchrotron radiation. Phenomena receiving particular attention include: (1) the Cooper minimum; (2) shape resonances; (3) autoionization; (4) correlation satellites; and (5) interchannel coupling. Systematic studies are being pursued on halogen acids, freons, nitrous oxide, and various metal vapors including Ag, Ga, Pb, and some 3d transition metal elements. Supportive calculations using the multiple scattering X Alpha method are being performed and correlated with observed cross sections and angular distribution parameters. Improved computer handling of the experiment has allowed the introduction of constant-ionic-state techniques. Besides providing fundamental information in atomic and molecular science, the program supplies data and ideas for studying molecules adsorbed on surfaces, clarification for solid state properties in metals, and an understanding of clusters. [2.6 FTE]

68. *Photochemical, Pyrolytic, and Reactive Intermediates By Electron Spin Resonance*
R. Livingston

Labile free radicals are observed at steady state concentration by ESR in circulating fluids at pressures up to 200 atm and temperatures to 700°C. Radicals are formed pyrolytically and photolytically with and without the use of added radical initiators such as peroxides. Work has centered largely on substances that are constituents of fuels and that are related to the production and combustion of organic fuels. Chemical product assays give additional information that is correlated with the kinetic parameters. Specific studies include properties of allyl radical and thermolysis of dibenzylamine. [0.3 FTE]

Sandia National Laboratories
Livermore, California 94550

Combustion Sciences Dept. **$5,260,000**

69. *Flame Dynamics Research*
R. Cattolica, W. Flower, S. Johnston

The purpose of this research is to investigate the spatial and temporal interactions between chemical species, temperature, and fluid motion as they occur in flames. Included in this work are the dynamics of carbonaceous particulates in sooting flames and the ignition, free propagation, and quenching of transient gas-phase flames. An important aspect of this work includes the development and application to flames of advanced optical diagnostics such as time-resolved, planar, laser-induced fluorescence, and diffusion broadening spectroscopy. Fluorescence imaging has been used to study the time-dependent interaction of a laminar flame with a single vortex, and the generation and evolution of the OH molecule during the interaction. Comparison of these results with the modeling predictions generated using the vortex dynamics computational method have been made. Soot size and number density, and the effect of increasing pressure on these quantities, have been determined in a laminar diffusion flame. Species thought to be responsible for soot particle surface growth have been detected using coherent anti-Stokes Raman spectroscopy. [3.0 FTE]

70. *Turbulent Reacting Flow Research*
R. Dibble, R. Schefer, S. Johnston

This research is directed toward an increased understanding of the coupling between the chemical kinetic and turbulent transport processes occurring in chemically reacting flows. The long-term goal is to use this understanding to improve predictive capabilities for turbulent combustion. Multi-species Raman concentration and temperature measurements, combined with simultaneous velocity determinations, have been compared with model predictions to estimate the influence of chemical nonequilbrium on mean turbulent flame quantities. A new laboratory incorporating a vertical flame tunnel (and making use of the CRF facility dye laser) is fully operational. A chemically reacting turbulent flow cooperative group comprised of participants from private industry, universities, and Sandia has been formed and meets on a regular basis. [3.0 FTE]

71. *Combustion Research Facility Operations and Visiting Scientist Support*
G. Drummond, D. Benthusen, R. Johnsen

This task supports all phases of Combustion Research Facility operations: (1) operation of the central Facility lasers; (2) operation and maintenance of the Facility VAX computer and networked minicomputers; (3) operation of the computer terminals to the Sandia CRAY; (4) staffing of the shop and analytical laboratories; and (5) maintenance of the safety and control system. This task also provides support for visiting scientists and for the transfer of technology developed and implemented at the Facility to others in the combustion community. Visitor support includes technician, scientific, engineering, and administrative staff dedicated to the visitors' project, as well as computer time, shop work, and purchases used directly by visitors or in support of them. The transfer of technology activity provides technical information to industry and university scientists through short courses in specialized areas, workshops on relevant topics, and combustion-related meetings and seminars. [13.0 FTE]

72. *CRF Diagnostics Research: Coherent Raman Processes*
R. Farrow, L. Rahn, R. Lucht, R. Palmer

This research effort is directed toward developing coherent Raman diagnostic techniques in support of Combustion Research Facility programs. New normalization techniques are being refined for coherent anti-Stokes Raman spectroscopy (CARS), a leading technique for time-resolved measurements of major species concentrations and temperatures. These new *in situ* normalization schemes provide accurate corrections to fluctuating CARS signals in high-pressure environments, and have been implemented in a CRF internal combustion engine experiment. The effects of Stark broadening and laser photon statistics on absolute concentration measurements are being explored. High-resolution inverse Raman spectroscopic measurements are providing precise high-temperature N_2 and CO lineshape data. The vibrational Stark effect discovered earlier is being quantified in a crossed-beam infrared absorption experiment to provide spatially precise CO spectra from a laboratory flame. [3.0 FTE]

73. *CRF Diagnostics Research: Advanced Methods*
J. Goldsmith, M. Koszykowski, F. Tully, R. Palmer

This project supports three broad areas of diagnostic research: (1) development of new multiphoton nonlinear techniques for detecting trace species in combustion environments; (2) research on advanced methods for kinetics studies; and (3) theoretical studies in support of CRF projects. In the first area, atomic hydrogen has been observed in a flame using multiphoton optogalvanic spectroscopy, representing the first direct *in* situ optical detection of this important radical in a combustion environment. Atomic oxygen and NO have also been studied with this technique. These methods are being used to map out H and O atom relative profiles in flat flames, and the capabilities and limitations for making absolute concentration measurements are being determined. Spatially resolved absorption methods are being developed for measuring other radicals in flames. Kinetics studies based on pulsed-laser photolysis followed by ultraviolet laser induced fluorescence have been extended to higher sensitivity by using a cw intracavity-doubled ring dye laser. Theoretical techniques involving electronic structure and scattering calculations, as well as approximate chemical kinetic theories, are being applied to a variety of CRF projects, including high-resolution spectroscopy, lineshape modeling, and kinetics studies. [3.0 FTE]

74. *Flame Chemistry: Modeling and Experiments*
W.J. McLean, J.A. Miller, M.D. Smooke, L.R. Thorne, R.W. Schmieder

The principal objective of this research is the development of comprehensive models for the chemical processes which govern flames. Emphasis is placed upon production and destruction of pollutants in flames. New numerical techniques have been implemented to provide fast and accurate methods for solving the one- and two-dimensional laminar flame equations, including sensitivity analyses, thereby facilitating comparisons with a wide range of experimental results. Laboratory studies emphasize the use of advanced laser probes for measurements of radical and stable species concentration profiles in flames. Other techniques, including molecular beam-mass spectrometry and Fourier transform infrared spectroscopy, are also employed.

During the past year, combined modeling and experimental studies were used to produce a comprehensive model for the conversion of HCN to N_2 and NO in flames. A detailed model for the structure and extinction limit of a methane-air counterflow diffusion flame was developed, and compared with experimental data. Experiments and computations are in progress to examine the chemical structure of premixed flames containing nitrogen and sulfur contaminants. Diffusion flame experiments using hydrocarbons labeled with carbon-14 at specific sites are being carried out to determine the propensity for particular molecular fragments to be incorporated into flame generated soot. [4.0 FTE]

75. *Chemical Kinetics and Dynamics*
W.J. McLean, F.P. Tully, R.A. Perry, D.W. Chandler, C. Melius

This research is directed at understanding fundamental chemical processes of importance in combustion. Laser photolysis is used to produce radicals in slow-flow reactors, and the kinetics and mechanisms of ensuing radical-molecule reactions are followed by chemiluminescence and laser induced fluorescence. Laser photoexcitation is used to produce energetic and reactive molecules whose subsequent chemistry (relaxation and reaction) is followed in time via state specific detection of products. Theoretical methods are also used to analyze pathways of combustion reactions. BAC-MP4 (Bond additivity corrected-Fourth order Moller-Plesset perturbation theory) calculations are used to determine the properties of stationary points (stable molecules and saddle points or transition states) on the potential energy surfaces of critical reactions. Statistical methods are used to predict rate coefficients and branching ratios from this potential surface information. In addition, the influence of inter- and intra-molecular energy transfer on unimolecular reactions is studied using dynamical methods. [4.0 FTE]

76. *CRF Central Laser Systems*
R. Schmitt, R. Farrow, R. Palmer

This project includes the continued development of existing CRF central lasers, and research in support of future major laser systems. The tunable dye laser, Diana, is operational, with performance levels which meet or exceed design specifications in all significant characteristics. Beam delivery and control throughout the Facility have been implemented. SNLL and visiting scientist experiments are now routinely using Diana. Possible system improvements include frequency doubling to obtain radiation from 240 to 370 nm, and mode-locking to obtain subnanosecond pulses. A new multipurpose laser system, Sirius, has been installed and used for CARS measurements in several different experiments. This new facility laser system, when fully completed, will provide serveral sources of high peak power, ultra-high resolution radiation, thereby adding CARS and other nonlinear spectroscopic capabilitites to all of the CRF laboratories. A third central laser consisting of a frequency-doubled pulsed Nd:YAG laser is being installed to provide additional capability to pump dye lasers in remote user laboratories. [3.0 FTE]

Atomic Physics

Argonne National Laboratory
Argonne, Illinois 60439

Division of Physics **$1,930,000**

77. *Photoionization Mass Spectrometry, Photoelectron Spectroscopy, and Photodissociation*
J. Berkowitz

Fundamental processes in the photoionization of atoms and small molecules are studied in the vacuum ultraviolet at high photon resolution. For molecules, alternative decomposition modes are investigated, providing important thermochemical values, structural and dynamical information. Photoelectron spectroscopy is focused on the more difficult high-temperature vapor species, and reveals their detailed electronic structure. A recently completed apparatus enables us to study directly the spectroscopy and dynamics of molecular-ion decomposition, by analyzing the decomposition products from interaction of UV-laser radiation with selected molecular ions. [3.9 FTE]

78. *Atomic Spectroscopy With Fast Beams At ANL*
H.G. Berry, L. Young

Measurements of $2s^3P_1$-$2p^3P_{0,2}$ transition wavelengths in highly-stripped two-electron atoms are continuing at the Argonne Tandem-Linac with ions of titanium. A new linear position-sensitive detector is being developed to replace the grating exit slits. A program of experiments utilizing laser excitation of fast ion beams has begun. Several experiments involving ion beam resonant excitation by collinear laser beams are under construction. Our first observations have been made of single photon and doppler-free two photon excitation in neon. An immediate goal is improvement of the accelerator voltage stability from 100 volts at present to less than 5 volts. Further measurements in hydrogen, helium, lithium, and sodium are in progress. Optical polarization measurements have been made of the light emitted from excited states of hydrogen and hydrogen-like helium following perpendicular and tilted carbon-foil excitation of protons, H_2^+ and He^+, at energies of 50-100 keV and 0.7 to 1.7 MeV. Strong alignment and orientation for highly excited states have been observed. They indicate a strong projectile-produced surface electric field of up to several mm in spatial extent. Beam-foil spectroscopy of multiply-excited states in light ions is continuing. We are also studying the fluorescence of atomic fragments of molecular ions following carbon foil break-up at Dynamitron energies. [4.4 FTE]

79. *Theoretical Atomic Physics*
K.T. Cheng

This program is directed toward a detailed understanding of the role of relativity and electron correlation in atomic processes. The emphasis is on photoexcitation and photoionization where one can gain important insight into the dynamics of many-electron interaction in atoms and ions. Current efforts include the systematic study of the ground-state hyperfine structures of rare-earth elements using a technique based on the multiconfiguration Dirac-Fock method. The same technique is used to study the fine and hyperfine structures of the Li^- ion which are very sensitive to Breit interaction and electron correlation effects. Studies are also being carried out on the changes in the correlation effect along an isoelectronic sequence as reflected in the profiles of the autoionization resonances. The purpose of this study is to gain better understanding of the dynamics of Rydberg series interactions. [1.1 FTE]

80. High-Resolution Laser-rf Spectroscopy With Atomic and Molecular Beams
W.J. Childs, L.S. Goodman

This program is directed toward a detailed understanding of interactions in atoms and small molecules. In the recent past the spin-rotation and hyperfine interactions of alkaline-earth monohalide radicals have been systematically studied and their dependence on vibrational, rotational, and isotopic effects elucidated. Within the last year the experimental methods have been extended to make possible measurement of the electric-dipole moments of such radicals. A similar program aimed at a systematic understanding of the hyperfine interaction throughout the 4f-shell of the rare-earth atoms is under way concurrently. A new apparatus for analogous studies of atomic and molecular ions using collinear laser and radiofrequency spectroscopy is under development. [3.1 FTE]

81. Interactions of Fast Atomic and Molecular Ions With Solid and Gaseous Targets
D.S. Gemmell, E.P. Kanter, Z. Vager

Argonne's 4.5-MV Dynamitron accelerator is used to study the interactions of fast (MeV) atomic and molecular ions with matter. A unique feature of the apparatus is the exceptionally high resolution (0.005° and 300 eV) in angle and energy obtained in detecting particles emerging from the target. The apparatus also permits the coincident detection of up to three molecular dissociation fragments. The work has as its main objective a general study of the interactions of fast charged particles with matter, with emphasis on those aspects that take advantage of the unique features inherent in employing molecular-ion beams (e.g., the feature that each incident molecular ion forms a tight cluster of atomic ions that remain correlated in space and time as they penetrate the target). In addition, we are able to study the structures of the molecular ions that constitute the incident beams. Current attention is being focused on the production of highly-excited Rydberg atoms formed in foil-excited ion beams. [4.9 FTE]

Brookhaven National Laboratory
Upton, New York 11973

Dept. of Physics **$255,000**

82. Atomic Physics Research
K.W. Jones, B.M. Johnson

Beams from the Brookhaven Double Tandem Van de Graaff Facility are used to study various aspects of ion-atom and ion-electron collisions. Energies for negative ions cover the range from about 1 to 9 MeV. Beams of almost fully stripped elements up to iron can be produced with energies from several MeV to several hundred MeV when the tandems are operated in the accel-decel and three-stage configurations. A lesser degree of ionization is obtained for heavier elements. Charge transfer and equilibrium charge states in ion-gas collisions are studied with negative ions, and with positive ions produced by the tandem accel-decel method. Inner-shell vacancy processes are also studied with these beams. An effort to measure electron ionization and excitation cross sections in an electron-heavy ion crossed-beam experiment is now in progress. Work to study the excitation and ionization of atoms and ions by photons from the National Synchrotron Light Source has been started. Design and fabrication of the beam line has commenced with first operation anticipated in 1984. Experimental apparatus for the initial experiments is currently being assembled. [3.1 FTE]

Lawrence Berkeley Laboratory
Berkeley, California 94720

Materials and Molecular Research Division **$410,000**

83. Atomic Physics
R. Marrus

This program is concerned with a broad-ranging experimental study of collisions and spectroscopy in simple atomic systems. Particular emphasis is placed on those processes pertinent to controlled thermonuclear reaction devices and processes important to fundamental physcial laws. Examples of such studies are: (1) electron capture by low-energy multicharged ions; (2) x-ray spectroscopy of heliumlike, lithiumlike, and berylliumlike ions of high Z; (3) parity violation in heavy atoms predicted by unified theories of weak and electromagnetic interactions; (4) charge capture and loss by fast multicharged atoms in solid and gas targets; and (5) study of quantum electrodynamic effects and relativistic effects in hydrogenic and heliumlike uranium. These studies take advantage of unique facilities developed within the group or available at LBL. Examples of such facilities are: (1) LBL's SuperHILAC and Bevalac that produce a range of heavy ion beams at energies greater than any other facility in the world; (2) ion trapping techniques developed within the group (making possible the application of this technique to more highly ionized states than have heretofore been achieved); and (3) narrow band, high-power UV lasers developed within the group for studying parity violation in atomic systems. [6.0 FTE]

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Physics Division **$1,240,000**

84. Theoretical Atomic Physics
R.L. Becker, C. Bottcher

Theoretical predictions, interpretations of experimental results, and detailed calculations are made for atomic collision, radiation, and structure phenomena. Emphasis is placed on reactions of highly stripped ions with atoms, particularly those reactions of importance in fusion energy devices and those studied in atomic high-energy accelerator physics laboratories. Atomic excitation, ionization, and electron transfer (capture) are treated. Recent activities include calculations of multiple K-, L-, and M-shell vacancy production by ions (being detected in x-ray satellites at the ORNL Holifield heavy ion accelerator), subshell vacancy production including the effects of vacancy rearrangement processes, electron capture and ionization in the nearly symmetric system F^{9+} + Ne at both low and high impact speeds, electron ejection and positron production in collisions of very heavy ions with very heavy atoms, and collisions of ions with atoms containing a highly excited (Rydberg) electron. New theoretical approaches include the one-and-a-half center version of coupled-channels theory, the unification of shakeoff theory with collision theory, and the use of finite elements in the numerical integration of time-dependent quantal equations. Computer programs for solution of the time-dependent many-electron Hartree-Fock and one-electron Dirac equations have been developed in the last year. [1.0 FTE]

85. Accelerator Atomic Physics
S. Datz, P.F. Dittner, P.D. Miller, C.D. Moak

The objective of this task is to achieve a detailed understanding of the interactions of high-energy, multiply charged, heavy ions with gas, solid, and electron targets. The primary facility used is the EN-tandem accelerator. Ion-ion collisions at low energies are also being investigated, and two experimental programs have been started on the Holifield accelerators. Examples of subjects which have received particular attention during the past year are: (1) cross section measurements of dielectronic recombination of O^{5+} and Cl^{6+} using a merged multiply charged ion beam concentric with an electron beam; (2) dependence of dielectronic recombination on stripping fields for C^{3+}; (3) transverse correlation effects on ion channeling trajectories; (4) production of polarized highly stripped ions by electron capture in ferromagnetic crystal channels; (5) mechanisms for transfer ionization; (6) continuing study of positron and electron channeling radiation; and (7) charge changing ion-ion collisions. Results in these areas impinge directly on fusion research, solar corona studies, and material sciences, as well as improving fundamental understanding of ion-atom, ion-solid, ion-ion, and ion-electron interactions. [5.9 FTE]

86. EN Tandem Operations
P.D. Miller, P.L. Pepmiller

The EN-tandem Van de Graaff is operated for atomic physics research. Terminal voltages up to 6.0 MV are routinely achieved, and ions of all elements from $Z=1$ through 9, and many heavier ions are available for users. The user group includes members of the physics division, other divisions of ORNL, faculty and students from various universities, and representatives from industry. During 1983, the installation of the Elbek spectrometer was completed. Calibration is now being done, and the first experiments will be undertaken during 1984. A new data acquisition system is being specified, and will be purchased and installed during 1984 and 1985. The major beam usage during 1983 was for the merged electron heavy ion beams experiments, convoy electron studies, trapping of low energy highly charged ions, and channeling experiments. Approximately 40% of the available beam time was utilized by university users. [1.6 FTE]

87. Collisions of Low-Energy Multiply Charged Ions
R.A. Phaneuf, H.F. Krause

This experimental program is aimed at improving our understanding of inelastic collision processes involving multiply charged ions at the lowest attainable collision energies. The current emphasis is on measurement of total cross sections for electron capture by highly stripped ions from hydrogen atoms at energies below 1 kev/amu. Toward this end, two different experimental approaches are being pursued. A pulsed-laser-produced plasma is utilized as a unique source of low-energy, highly stripped ions which are directed through a calibrated thermal-dissociation atomic hydrogen gas target. Charge and energy analysis is effected by a time-of-flight technique. Total electron-capture cross sections have been measured recently for B^{+q} ions ($2 \leq q \leq 5$) at energies in the range 10-100 eV/amu, and provide data for testing predicted ionic charge scalings at low energies. An ion-atom merged-beams apparatus is also in final stages of development and testing. This will permit study of such collisions at center-of-mass energies as low as 1 eV/amu, where theoretical predictions of increasing cross sections with decreasing energy remain untested. [1.4 FTE]

Sandia National Laboratories
Albuquerque, New Mexico 87185

Dept. of Laser R&D **$155,000**

88. Atomic Processes
A. Owyoung, J.P. Hohimer, A.V. Smith

This research is directed toward the study of high-order nonlinear optical interactions in atomic and molecular systems, with the goal of uncovering an efficient method for the generation of fully tunable coherent vacuum ultraviolet (VUV) radiation. Present investigations are concentrating on fifth-order, two-frequency summing processes in atomic vapors whereby third harmonic generation at one frequency is enhanced by a second laser source, which effectively couples the process into a four photon resonance with the atomic system. Our investigations will continue to explore phenomena involving such "optically induced structure" in the continuum between states, but will also be extended out to the ionization continuum. These subsequent studies will both extend the accessible VUV tuning range and provide for the exploration of more complex interactions that are expected to occur when resonant ionization becomes a significant consideration. This research project will not only provide a new and potentially very useful means for VUV generation, but also contribute significantly to our understanding of the complex interactions of optical radiation with atomic and molecular systems. [1.5 FTE]

Chemical Energy

Ames Laboratory
Ames, Iowa 50011

Processes and Techniques **$1,006,000**

89. Organometallic Complexes in Homogeneous Catalysis
R.J. Angelici

The major thrust of this research is to understand the role of organometallic complexes in transition metal-catalyzed reactions and to seek new catalytic reactions that provide energy-efficient routes to useful chemicals. Of particular interest are reactions of ethylene oxide with CO. It has been demonstrated that CO ligands in complexes of Fe, Ru, Mn, and Re react with ethylene oxide to form dioxo-carbene complexes of those metals. This type of reaction is being examined for possible catalytic applications. In another area, possible mechanisms for the hydrodesulfurization (HDS) of thiophene are being investigated by studying the reactivity of π-bonded thiophene in transition metal complexes. Early results indicate that the coordinated thiophene is highly activated to react with transition metal hydrides, a possible reaction occurring on heterogeneous HDS catalysts. [2.7 FTE]

90. *Chemical Kinetics and Reactivity of Transition Metal Complexes*
J.H. Espenson

Organometallic complexes such as $(H_2O)_5Cr\text{-}R^{2+}$, $R\text{-}Co(dmgH)_2L$, and $R\text{-}Rh(dmgH)_2L$ are under active investigation, as are dinuclear compounds having a metal-metal bond. The research concerns the reactions which occur and their kinetics and mechanisms, especially reactions in which the metal-carbon bond is formed or broken, or in which the organic group, R, reacts further. Novel displacements by free radicals are being investigated using techniques such as stopped-flow kinetics, product competition ratios, stereochemical labeling, and flash photolysis. Included are classes of compounds important in Fischer-Tropsch reactions, such as α-hydroxyalkyls. Studies of metal-carbon bond homolysis permit: (1) evaluation of therymodynamic bond dissociation energies; (2) resolution of the mechanism of homolytic cleavage vs. competing heterolysis; (3) examination of novel free radical displacement reactions; and (4) evaluation of the kinetic reactivity of aliphatic radicals. Conditions have been developed for the use of metal complexes to generate aliphatic radicals in solution in a controlled manner. Mechanistic studies are also in progress to learn how insertions into metal-metal bonds to form molecular A-frames occur, and to study the reactivity of such compounds. [4.9 FTE]

91. *Nuclear Magnetic Resonance (NMR) Studies of Coals, Catalysts, and Amorphous Semiconductors*
B.C. Gerstein

Solid state NMR is used to infer chemical functionality in coals and products of coal conversion (e.g., solid asphaltenes) and to probe hydrogen, silicon, and aluminum in zeolites used for converting methanol to ethylene. In addition, the morphology of proton containing regions in amorphous silicon-hydrogen alloys, and the types of SiH_x groups present in these materials are studied by solid state proton and silicon NMR using a variety of experiments involving the proton and silicon spin dynamics. [4.0 FTE]

92. *Spectroscopic and Kinetic Characterization of Metal Oxide and Sulfide Catalysts*
G.L. Schrader

The goal of this research is to develop a fundamental understanding of the solid state and surface chemistry of heterogeneous catalysts and the mechanisms of catalytic reactions. Metal oxide and sulfide catalysts for producing synthetic fuels or for hydrotreating coal-derived liquids are being investigated; catalysts for energy-efficient routes to chemicals are also important in this research. Spectroscopic techniques such as laser Raman spectroscopy and Fourier transform infrared spectroscopy are being used to characterize catalysts and adsorbed species. *In situ* experiments are being performed involving functioning catalysts; simultaneous spectroscopic and kinetic measurements can be performed at temperatures and pressures typical of industrial operating conditions. These techniques provide a direct method for relating structure and composition to catalytic activity, selectivity, and stability. The effects of defect structures, oxidation state, and nonstoichiometry are particularly important for the metal oxide and sulfide catalysts being examined. Adsorption and reaction studies are being performed using pulsed and steady-state fixed bed reactors. [1.9 FTE]

93. *High-Temperature Gas-Phase Pyrolysis of Organic Compounds*
W.S. Trahanovsky

This research is directed toward an understanding of the fundamental thermal reactions of organic compounds, especially those that could be important in the pyrolysis of coal and coal-derived liquids. The work can be divided into three main categories: (1) determining the major pyrolysis reactions of model compounds; (2) preparing and studying physical and chemical properties of reactive compounds thought to be intermediates in pyrolysis reactions; and (3) determining the importance of surface-catalyzed reactions under various pyrolysis conditions. Most pyrolyses are carried out using the flash vacuum pyrolysis technique. Much of the work concentrates on the study of pyrolysis reactions that are thought to involve quinodimethanes as intermediates, on preparing and characterizing these and related species, and on thermal reactions of these species and products derived from them. Specific compounds under study include tetralins, 2,3-dimethylene-2,3-dihydrofurans, the furan and thiophene analogs of *ortho*-quinodimethanes, and benzocyclobutenes, and the closed forms of *ortho*-quinodimethanes. [2.2 FTE]

94. *Study of Solid-Gas Reactions Which Involve Structural Changes In the Solid*
D.L. Ulrichson, A.H. Pulsifier

The objective of this project is to understand and describe the behavior of the class of solid-gas reactions which exhibit either expansion or contraction of the solid during reaction. In the case of solid expansion, the increased volume of the solid product closes diffusion paths for the gaseous reactant and stops the reaction at less than total conversion. The reaction of sulfur dioxide with calcium oxide (used to remove sulfur dioxide from boiler flue gas) is an example in which only about thirty percent of the calcium oxide reacts before the reaction stops. Previous models concentrated on the effect of the reduced porosity resulting from product expansion. Data from this project indicate that diffusion of reactant through the solid product layer is as important as pore reduction. Inconsistencies in published results for several solid-gas reactions can be explained by including this term. Current work emphasizes measurement of diffusion rates through the pores and through the solid product layer. [0.5 FTE]

Argonne National Laboratory
Argonne, Illinois 60439

Division of Chemical Technology	**$468,000**

95. *Fluid Catalysis*
J.W. Rathke, M.J. Chen, R.J. Klingler, J.J. Heiberger

This research attempts to determine reaction mechanisms and to develop new catalytic chemistry for converting small molecules (e.g., CO and CO_2) to specific desired products. Currently under investigation are the roles of formate and carbonate ions in the mechanism of operation of a new series of catalysts for reacting carbon monoxide with water or hydrogen to produce alcohols. The new chemistry is unusually general in that it applies to both main group and transition metal centers. Related to this study is an investigation of the precise chemical transformations involved in the activation of hydrogen, carbon monoxide, and carbon dioxide by homogeneous and heterogeneous metal oxide complexes. Also studied is the role of alkali metal promoters in converting methanol to higher alcohols in catalytic alcohol syntheses. The mechanisms of these reactions are being investigated using a combination of high-pressure kinetic, spectroscopic, and theoretical (molecular orbital) methods. [5.3 FTE]

Division of Chemistry **$1,715,000**

96. *Inorganic Fluorine Chemistry*
E.H. Appelman, L.J. Basile, L. Stein

This program has as its objective the synthesis and characterization of novel inorganic oxidants and fluorinating agents, as well as the development of applications of these exotic compounds to other areas of chemistry. Ongoing work includes thermodynamic characterization of SO_4F^- and HSO_5^-, evaluation of the acidities of strong acids in anhydrous HF, the use of noble gas compounds to aid the characterization of low-temperature matrices by EXAFS spectroscopy, exploration of the interaction of F_2 with aqueous solutions, the application of SO_4F^- as a fluorinating reagent for organic and organometallic chemistry, and the study of hydrolytic reactions of radon compounds. [2.4 FTE]

97. *Premium Coal Sample Program*
K.S. Vorres

The objective of this program is to provide the U.S. basic coal science research community with long-term supplies of a small number of premium coal samples. The premium coal samples produced and distributed by this program are to be as chemically and physically identical as possible, have well-characterized chemical and physical properties, and be stable over long periods of time. Coals are to be mined, transported, processed into desired particle and sample sizes, and packaged in environments which are as free of oxygen as possible and which maintain the natural moisture content to insure that the coals are kept in as pristine and stable condition as possible. These premium samples are to be distributed to researchers upon request. It is anticipated a computer data base will be included in this program to provide researchers with easy access to detailed information on sample availability, the physical and chemical properties of the coals, and references to the results of research obtained using these samples. [3.6 FTE]

98. *Fundamental Chemistry of Coals and Other Fossil Fuels*
R.E. Winans, R. Hayatsu, R.E. Botto, R.G. Scott, R.M. McBeth

As its major objective this program seeks to provide a fundamental understanding of the organic structures in coal and coal macerals and to be able to relate this information to the reactivity of these materials. Synthetic coal macerals are being prepared in a unique process. This study provides insight into how macerals are formed and yields well-characterized macromolecular models for coals. Selective chemical reactions, pyrolysis MS and solids NMR are used for characterization of both synthetic and natural macerals. New separations and identification techniques for large and nonvolatile molecules are being developed for this program. [7.2 FTE]

Brookhaven National Laboratory
Upton, New York 11973

Dept. of Applied Sciences **$588,000**

99. *High Temperature Chemistry*
J.J. Egan

This study of the thermodynamic and transport properties of inorganic substances at high temperatures attempts to explain the results in terms of appropriate atomic models. Substances include solid and liquid compound semiconductors, solid electrolytes, and molten salts. Electrochemical techniques are used to investigate the effect of composition on the concentration, mobility, and diffusion of electrons and electron holes in these substances. Cells employing solid electrolytes at high temperatures as well as molten salt electrolytes prove especially useful for characterizing these systems. High temperature calorimetry is being used to study liquid semiconductors and other liquid alloy systems. Molten salts are studied since they are important for the development of high energy-density batteries and fuel cells. The electronic conductivity of these melts in particular is examined by special techniques. Solid compound semiconductors of potential use as solar cells are studied by high temperature electrochemical techniques. [2.2 FTE]

100. *Metal Hydrides*
J.J. Reilly

The overall concern of this program is the determination of the thermodynamic properties and structural parameters of metal alloy-hydrogen systems. Particular goals are to relate hydriding properties of metal alloys to their structure and composition, determine alloy-hydrogen phase diagrams, determine and systematize crystal structure and, finally, relate all pertinent data and observations for a predictive capability of the behavior of a given alloy-hydrogen system. Current topics of interest are the causes of the observed deviations from ideal behavior of certain intermetallic-hydrogen systems, surface and near surface properties of metal-hydrogen systems, the partial molar volume of hydrogen in intermetallic compounds, the influence of defects upon system behavior, and reaction kinetics of metal hydride suspensions. The major experimental tools and/or techniques consist of x-ray and neutron diffraction, equilibrium pressure temperature composition measurements, ion beam analysis, and magnetic susceptibility measurements. [4.1 FTE]

Dept. of Chemistry **$416,000**

101. *Organometallics in Homogeneous Catalysis*
M.A. Andrews

The major emphasis of this project is the development of a better understanding of the role that soluble transition metal complexes can have in the homogeneous catalytic oxidation of organic substances. A potential long term benefit of this work includes the discovery of more efficient alkene epoxidation catalysts. The approach currently under investigation takes advantage of the fact that transition metal nitrosyl complexes can symmetrically cleave atmospheric dioxygen to give metal nitro complexes. These species can then transfer an oxygen atom from the nitro group to an alkene substrate to give epoxides and other oxidized products. The mechanism of alkene oxidation by $Pd(CH_3CN)_2ClNO_2$ has been studied in detail, primarily through the isolation ~~and characterization~~ of intermediates (alkene and heterometallacyclopentane complexes) and the analysis of product distributions as a function of the alkene substituents and stereochemistry. Future studies will be devoted to the investigation of other metal nitro catalyst systems, the development of oxygen atom carriers besides nitro groups, and more detailed studies of the factors governing the selectivities of these systems for epoxides vs ketones and other beta-hydrogen elimination derived products. [4.2 FTE]

102. *Mechanisms of Photo-, Enzyme-, and Chemically Catalyzed Cis-Trans Isomerization*

S. Seltzer

Cis-trans isomerization can be brought about by the application of heat or light, or by catalysts. Because the physical and chemical properties of the two isomers differ, relaxation of a nonthermodynamic mixture of isomers (achieved by irradiation) to the thermodynamic mixture can result in the release of thermal or electrical energy. This cis-trans energy-producing effect is utilized in biological processes such as vision in animals and the light-driven proton pump of Halobacteria, which can be used in a photogalvanic cell. Studies at BNL are concerned with mechanisms of cis-trans isomerization catalyzed by chemical reagents, by enzymes, and by light, and their applications to the mechanism of the bacteriorhodopsin proton pump. [1.5 FTE]

DOE/Pittsburgh Energy Technology Center
Pittsburgh, Pennsylvania 15236

Analytical Chemistry Branch **$93,000**

103. *Vibrational Spectroscopic Studies of Coal Conversion Catalysts*

J.M. Stencel

Research during the current year has concentrated on understanding molybdenum-support and tungsten-support interactions in Mo/Al_2O_3, W/Al_2O_3, $Ni\text{-}Mo/Al_2O_3$, and $Ni\text{-}W/Al_2O_3$ catalysts. Raman spectroscopy is the primary tool used to define molecular speciation for catalysts in which Mo, W, and Ni concentrations have been varied systematically. Additional information concerning the influence of concentration and symmetry of the metal oxides on their vibrational frequencies is obtained by *in situ* experimentation and by adsorption of ligand-forming and hydrogen-bonding molecules. Raman experimentation is supplemented by data from other bulk and surface sensitive techniques such as x-ray diffraction, x-ray photoelectron spectroscopy, and ion scattering spectroscopy. Correlations are made with catalytic reaction data to provide insight into structural and chemical factors that influence catalytic activity. [1.0 FTE]

Lawrence Berkeley Laboratory
Berkeley, California 94720

Applied Science Division **$32,000**

104. *Bioconversion of Cellulose*

C.R. Wilke, H.W. Blanch

This project investigates primarily the enzymatic hydrolysis of biomass to hexose and pentose sugars. Basic information on the kinetics and mechanism of enzymatic hydrolysis is to be obtained. This information can then be used to develop low-cost processing schemes for sugar production. High productivity fermentations to convert these sugars to ethanol or other chemical feedstocks are being developed. Fundamental studies on yeast metabolism in high cell density cultures will be obtained. This will be combined with basic studies on ethanol separation from the fermentation broth, using novel, low-energy solvent extraction schemes. [2.0 FTE]

Materials and Molecular Research Division **$1,300,000**

105. *High Energy Oxidizers and Delocalized-Electron Solids*

N. Bartlett

The program's main aim is the synthesis and characterization of new materials. The synthetic work tests models and theories which correlate physical properties (such as electrical conductivity) with chemical composition and structure. Emphasis is on the study of two-dimensional extended atomic networks such as those derived from graphite, layer-form boron nitride and their relatives. Electron-oxidation of such materials (with accompanying intercalation to form salts) generates durable and conductive materials (some better than aluminum). Chemical, stoichiometric, and structural requirements for the best conductivity are being defined. Layered materials can often be oxidized (and intercalated) electrochemically, the process also being reversible. Thus graphite may be reversibly converted by electrochemical means to a graphite flouride of approximate composition $C_{2.5}F$. This novel material, which could be important as a high-energy electrode, possesses a π-electron system which appears to be similar to that in pristine graphite. Physical and chemical studies are being applied to this and related materials to determine the structure and bonding changes which accompany the oxidation and reduction. Salts which are either proton conductors or flouride ion conductors, but not metallic, and which are resistant to oxidation, are being sought as solid electrolytes for use with metallic layer-material salts. [4.7 FTE]

106. *Catalytic Hydrogenation of Carbon Monoxide*

A.T. Bell, G.A. Somorjai

The purpose of this program is to develop an understanding of the fundamental processes involved in catalytic conversion of carbon monoxide and hydrogen to gaseous and liquid fuels. Attention is focused on defining the factors which limit catalyst activity, selectivity, and resistance to poisoning, and the relationship between catalyst composition/structure and performance. To meet these objectives, a variety of surface diagnostic techniques (LEED, AES, XPS, EELS, IRS, TPD) are used to characterize supported and unsupported catalysts before, during, and after reaction. The information thus obtained is combined with detailed studies of reaction kinetics to elucidate reaction mechanisms, and the influence of modifications in catalyst composition and/or structure on the elementary reactions involved in carbon-monoxide hydrogenation. [6.0 FTE]

107. *Transition Metal Catalyzed Conversion of CO, NO, H_2*, and Organic Molecules to Fuels and Petrochemicals

R.G. Bergman

The central objective of this program is the discovery of new chemical reactions between organic compounds and transition metals, and the understanding of how these reactions work. Particular attention is paid to transformations that involve the most fundamental bonding changes (e.g., formation and cleavage of bonds between carbon, hydrogen, nitrogen, and oxygen), which occur in important large-scale transformations of organic compounds, such as those employed in industrial catalysis and stoichiometric organic synthesis. A recent discovery on this project was that a certain class of iridium complexes undergoes oxidative addition into the carbon-hydrogen bonds of completely saturated hydrocarbons (alkanes). This is the first example of this long sought C-H activation reaction, and research during the past year has been directed at understanding its scope and selectivity. Recently, methods for extending the iridium-based alkane activation chemistry to appropriately substituted rhodium complexes have been developed. Work is under way aimed at studying the properties of these different metal systems, understanding and comparing the mechanisms of the reactions, and developing methods for using this chemistry to convert alkanes into more useful, functionalized organic molecules. [2.6 FTE]

108. *Formation of Oxyacids of Sulfur From SO_2*

R.E. Connick

The research is aimed at understanding the fundamental chemistry of sulfur species formed from sulfur dioxide in aqueous solution and the chemical reactions of these species. The chemistry of these systems is of particular importance in the problems associated with atmospheric pollution by sulfur dioxide and the resulting formation of acid rain. Research has focused on the kinetics of the exchange of oxygen atoms between bisulfite ion and water, using the nuclear magnetic resonance of oxygen-17 for following the reaction. Results indicate a rate law consistent with exchange through formation of sulfur dioxide. The most intriguing finding is that there are two separate bisulfite species present, presumably the two isomers, which differ in the attachment of the proton to the oxygen or the sulfur. The latter species is about one-sixth as abundant as the former and does not exchange oxygens with water at a significant rate. A secondary and not closely related goal is to determine the factors controlling the rate of substitution reactions in the first coordination sphere of metal ions. Computer modeling of such systems is under way and some results for a two-dimensional model have been published. Work will be extended to three dimensions using a more sophisticated model for water. [2.0 FTE]

109. *Chemistry and Morphology of Coal Liquefaction*

H. Heinemann

We are studying the catalytic gasification of graphite or char to produce methane and higher hydrocarbons. Within the last year it has been found that the apparent self-limiting step, namely the formation of a potassium phenolate group, can be circumvented by a simultaneous catalytic decomposition of the phenolate. It is intended to now look for better catalysts for this step and to improve rates and yields of hydrocarbon formation as well as to determine the mechanism for the formation of hydrocarbons heavier the C_1. In the selective hydrogenation of nitrogen-containing aromatics, work is under way to find methods for splitting out N as nitrogen or ammonia from partly-saturated aromatics. (If successful, this would provide leads for a low-temperature, low-pressure denitrification with low hydrogen consumption.) Simultaneously, catalytic mechanisms of hydrogen tranfer from partially-saturated, nitrogen-containing ring compounds are being investigated. [1.2 FTE]

110. *Synthetic and Physical Chemistry*

W.L. Jolly

The main objective of this project is to determine the nature of the chemical bonding in transition-metal organometallic complexes related to catalytic systems. The experimental tool is gas-phase x-ray photoelectron spectroscopy, which provides atomic core electron binding energies. The binding energies give information about the distribution of valence electron density and the nature of the chemical bonding in the molecules. By measuring the core binding energies of appropriate transition metal compounds, it is possible to study the interaction of metal d electrons with various ligands, such as organic groups, carbonyl groups, and nitrosyl groups. One can identify and distinguish various modes of ligand metal bonding which have analogs in the molecules chemisorbed on metal surfaces and in the intermediates of catalyzed organic reactions. Of particular interest are studies of metal cluster complexes, in which the ligand-metal interactions are very similar to those on metal surfaces. [1L1.5 FTE]

111. *Surface Chemistry–Application of Coordination Principles*

E.L. Muetterties

Definition of the coordination chemistry of transition metal surfaces on a comparative basis with that of molecular metal complexes and molecular metal clusters is the research objective. Displacement reactions, supplemented with diffraction and spectroscopic data, will be used in elucidation of structural, bonding, and chemical features of the nickel and platinum metal surfaces with chemisorbed molecules. Initial studies focused on the chemisorption states of aromatic hydrocarbons, olefins, and acetylenes on nickel and platinum surfaces. Catalytic reactions of these molecules will be examined in an ultrahigh vacuum chamber equipped with an isolation cell. These catalytic reactions will be closely correlated with metal cluster research so as to obtain a precise comparison between homogeneous and heterogeneous catalysis. Theoretical analysis, based on symmetry matching of energetically available metal surface orbitals with those of molecules and molecular fragments of hydrocarbon, has been developed for a further comparison with structural data. [2.0 FTE]

112. *Electrochemical Systems*

J. Newman

This program includes investigation of fluid flow and electrochemical transport, analysis of mass-transfer rates and current distribution, design of practical electrochemical systems, and investigation of corrosion processes. Coupled kinetic, mass-transfer, and fluid-flow phenomena are investigated in semiconductor electrode systems, with emphasis on the optimization of configurational and operating parameters of liquid-junction photovoltaic cells. [0.4 FTE]

113. Organometallic Chemistry of Coal Conversion
K.P.C. Vollhardt

The basic program objective is to apply organometallic processes and techniques to the solution of problems concerned with the conversion of coal to liquid and gaseous fuels. The potential of novel organometallic systems as catalysts and photostorage devices is being explored. A series of experiments on trinuclear biscarbyne clusters as potential models for surface mediated carbon-carbon and carbon-hydrogen bond making and bond breaking processes has been completed. This work has led to the discovery of novel transformations in the coordination sphere of transition metal clusters including carbyne-carbyne coupling and decoupling, chalcogen induced degradation, and electrophillic substitution chemistry at the apical carbon. In addition, a novel thermally reversible photochemical vinyl-hydrogen activation has been observed with potential in photochemical storage devices. A new method for constructing fulvalene complexes has allowed the exploitation of unprecedented binuclear chemistry of homo- and heteronuclear transition metal derivatives. Several of these compounds have shown novel and distinct chemistry of relevance to catalysis and photochemical storage cycles. These systems are being investigated as potential models in heterogeneous Fischer-Tropsch polymerization and the activation of small molecules. The preparation and isolation of soluble, defined molecular systems has allowed structural and mechanistic information to be assembled in unprecedented material. [2.4 FTE]

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Chemistry Division **$234,000**

114. Synthesis of Thermochemical Cycles
W.M. Jones, E. Onstott, M. Bowman

This research is directed to an understanding of the basic chemistry and engineering principles required to synthesize efficient thermochemical cycles for the production of hydrogen from water by the use of heat sources such as solar, nuclear fission, and nuclear fusion reactors. A general objective is to establish the criteria required for the development of this new technology and for the evaluation of worldwide programs. The research consists of the identification, initial evaluation, and preliminary development of different cycles through measurements of reaction rates, reaction yields, and thermochemical properties. Current studies include: (1) thermochemical cycles based on decomposition of metal sulfates and hydrogen iodide, where the recycle reagents are sulfur dioxide, water, iodine, and a rare earth dioxymonosulfate; and (2) evaluation of low temperature reactions in cycles based on decomposition of metal oxides and hydrogen iodide, where the recycle reagents are water, iodine, magnesium hydroxide, and an oxide of copper, iron, manganese, or cobalt. [1.4 FTE]

Isotope and Nuclear Chemistry Division **$235,000**

115. Labile SO_2 Complexes
G.J. Kubas, G.D. Jarvinen, R.R. Ryan

The basic chemistry of sulfur dioxide is being expanded with regard to its binding to transition metal complexes, enhancing its reactivity and promoting catalytic reactions. The ultimate goal is development of new methods for scavenging SO_2 from flue-gases. Work includes synthesis and structural characterization of new SO_2 complexes and catalytic reactions of SO_2 with other small molecules. For example, SO_2 and NO_x have been converted to sulfur, nitrogen, and water by hydrogen reduction over a Ru/alumina catalyst, and methods of catalyzing such reactions homogeneously are being investigated. A catalytic conversion using organometallic molybdenum sulfide complexes has been discovered in which hydrogen reduction of SO_2 to sulfur and water takes place under mild conditions. Reactions of SO_2 with transition metal hydride complexes are being studied in order to identify intermediates and mechanisms involved in hydrogen transfer to SO_2, and insertion of SO_2 into a metal-hydride bond, a possible key step in hydrogenation, has been observed for the first time. As a spinoff of the above work, the first example of a molecular hydrogen complex, $W(CO)_3(PR_3)_2(eta^2\text{-}H_2)$ has been discovered, and its possible role in catalytic hydrogenation is under investigation. [1.5 FTE]

Monsanto Research Corporation
Miamisburg, Ohio 45342

MRC-Mound **$175,000**

116. Fundamental Investigations Of Metal Hydrides
R.C. Bowman, Jr., G.C. Abell, M.P. Guse

The program objective is to obtain a fundamental understanding of the role of interstitial hydrogen on the electronic and structural properties of a host metal. Experimental techniques such as NMR, variable temperature x-ray diffraction, and thermal analysis are being used: (1) to evaluate specific properties of the electronic structure; (2) to determine the effect of host metal structure, hydrogen site occupancy, and alloy substitution on hydrogen diffusion; and (3) to study the ramification of phase transitions on the electronic structure of the metal hydrides. Among the hydrides under current investigation are the AB_5 compounds, zirconium and titanium based alloys both crystalline and amorphous, and the Laves alloys. Monte Carlo type calculations are used to correlate NMR lineshapes with hydrogen site occupancy. Quantum-mechanical calculations of the electronic properties of clusters of metal atoms with hydrogen interstitials are being used to describe additional experimental results. Short-range electronic structures are being explained using a localized electronics states model. [2.5 FTE]

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Chemical Technology Division **$310,000**

117. Kinetics of Enzyme Catalyzed Processes
E. Greenbaum, J. Woodward

This research project is focused on understanding the fundamental chemical and physical mechanisms of enzyme-catalyzed reactions. The specific systems under investigation are the *in* vitro photosynthetic system composed of isolated chloroplasts, ferredoxin, and hydrogenase (CFH), and the enzyme-catalyzed conversion of cellulose to glucose. The CFH system is capable of the simultaneous photoproduction of hydrogen and oxygen when irradiated with visible light. Experimental progress includes the first measurements of the light saturation curves of biophotolysis of water and the first demonstration of the simultaneous photoproduction of hydrogen and oxygen by immobilized chloroplasts, ferredoxin, and hydrogenase. The result is that the analytical shapes of the light saturation curves are not the same. A higher light intensity is required to saturate the hydrogen curve. These results challenge the Z-scheme concept of photosynthesis. A cellulase enzyme system is being investigated for the conversion of cellulose. An immobilized enzyme has been shown to maintain long-term stability and high activity for this application. [3.0 FTE]

Chemistry Division **$2,183,000**

118. Basic Aqueous Chemistry to High Temperatures and Pressures

H.F. Holmes, W.L. Marshall, R.E. Mesmer, D.A. Palmer, J.M. Simonson

Research is conducted to derive an understanding of the principles controlling homogeneous and heterogeneous chemical processes to the extreme conditions (pressure-temperature-compositions) encountered in technological and natural systems. Advancement in techniques and in existing unique equipment will continue to be emphasized in studies of the reaction types: association, ionization, oxidation-reduction, hydrolysis, hydration, complexation, and precipitation. Species identification, thermodynamic properties, and equilibrium stability information are obtained, but new emphasis will be placed on structural and detailed quantitative information from neutron and Raman scattering research in collaboration with other programs in the Division. The future goals of the group include extension of the P-T-X conditions attainable in studies of excess Gibbs energies and enthalpies for important electrolyte systems, as well as definitive work on conductivities, electrochemical cells, and solution flow calorimetry. New techniques will be developed for studies of volumetric properties, absorption spectrophotometry, Raman spectroscopy, and neutron scattering. Results will contribute to the advancement in theories and models for water and its solutions, as well as provide a basis for detailed descriptions of the chemistry for systems important to steam generation, nuclear coolants, geochemical and hydrothermal processes, waste transport, nuclear accident assessment, and supercritical fluid processing. [5.5 FTE]

119. Heterogeneous Catalysis Related to Energy Systems

S.H. Overbury, D.R. Huntley

This program involves two related activities. In the first, the technique of low energy ion scattering as a surface specific structural tool is being developed and applied to the study of clean and adsorbate covered surfaces of catalitic interest. Comparison of the experimentally observed energy and angle dependencies of the scattered ions with computer simulations allows for quantitative descriptions of surface structure. The information content from alkali metal ions (Li^+, K^+) exceeds that from inert gas ions because of their lower neutralization probability. These methods have been applied to study surface reconstruction of Au(110), bonding geometry and ordering of O, C, N, and S overlayers on Mo(001), and surface structure of amorphous $Fe_{80}B_{20}$ ribbon. The second activity, under initial development, will examine surface adsorption on metal sulfide surfaces in ultrahigh vacuum by electron spectroscopy and by thermal desorption spectroscopy. A sample transfer system will permit the sample to be moved to an adjoining high pressure cell, which will be used for monitoring hydrodesulfurization and hydrogenation reactions over a wide pressure range. Measured reactivity and selectivity will be correlated with changes in the surface modified by introducing structural defects, bulk or surface impurities, or changes in stoichiometry. [2.3 FTE]

120. Organic Chemistry and the Chemistry of Fossil Fuels

M.L. Poutsma, B.M. Benjamin, L.L. Brown, E.W. Hagaman, R.R. Chambers

The objective of this program is improved understanding of the chemical structure and reactivity of coal. The approach involves chemical and spectroscopic techniques, and interpretation of results from studies with coal is aided by parallel studies with appropriate model compounds. The key spectroscopic technique used for native and chemically modified coals is solid-state CP/MAS ^{13}C NMR. Current emphasis is on developing reliable techniques for quantification, and a recent initiative is aimed at performing double cross polarization experiments. Diagnostic reactions for structural features in coal are being developed, including the selective derivatization of coal carbanions based on differences in acidity of C-H bonds, and the identification and quantitation of aliphatic substituents and linking groups in coal by acid-catalyzed transalkylation. The effect of diffusional restraints on the thermal reaction pathways of key structural units in coal is investigated by the use of model compounds covalently attached to the surfaces of inert solids. [8.3 FTE]

121. Molten Salt Catalysts For Clean Fuel Synthesis

G.P. Smith, A.C. Buchanan, III, A.S. Dworkin, S.P. Zingg

This research is directed at the mechanisms by which molten halide salts hydrocrack coal model compounds. Our study of the important redox functionality of antimony trichloride-based catalysts continues and is now focused on the formation and decay reactions of radical cations and dications of polycyclic arenes and heteroaromatics in these media. We recently demonstrated that redox functionality is an important component of the catalytic activity of gallium trichloride in which the uncomplexed gallium(I) ion provides the reduced state. We will soon begin studies to determine whether or not aluminum chloride and the chloroaluminates possess a redox functionality. These investigations are based on the application of *in situ* spectroscopies (NMR, ESR, and fast optical) and electroanalytical methods combined with quench and separation procedures. Highly purified salts are used in controlled atmosphere glove boxes and closed systems. [4.7 FTE]

Pacific Northwest Laboratories
Richland, Washington 99352

Dept. of Chemical Technology **$470,000**

122. Hydrogenation Mechanisms of Coal

J.A. Franz, R.D. Barrow, D.M. Camaioni

This program is basic research directed at determining the energetics and mechanisms of free radical reactions related to thermal dissolution of coal in hydrogen donor media. Relative rates of radical rearrangements, atom transfer reactions, fragmentation reactions, and charge transfer reactions are being determined, with absolute rates determined by kinetic laserflash spectroscopy for key atom transfer reactions. The cyclization of ortho-allylbenzyl radical to 2-indanylmethyl radical, for example, is used as an intramolecular free radical clock to compare atom transfer rates to benzylic radicals, thereby determining the relative donor strength of a wide variety of coal-related donors. [2.0 FTE]

123. Thermochemical Conversion of Solid Wastes Into Liquid Fuels
D.A. Nelson, P.M. Molton, R.T. Hallen

The purpose of this research is to determine the reaction mechanisms involved in biomass liquefaction in aqueous media at elevated temperatures. Due to the complexity and variability of the composition of biomass, the liquefaction of pure cellulose is now being studied. Fast heating and cooling during liquefaction has helped determine which components are initially produced from cellulose. For instance, biacetyl appears to be formed from erythrose which is a retro-aldol product of glucose. Thus, many of the reactive intermediates formed during liquefaction act as precursors for other products with time. The use of alkaline catalysts under liquefaction conditions was to shift the mechanism from one involving aqueous pyrolysis (predominant furan formation) to one incorporating aldol and related condensations. Incomplete mixing of the alkaline catalyst allowed both mechanisms to operate during liquefaction with fast heating and cooling rates. [1.8 FTE]

Sandia National Laboratories
Albuquerque, New Mexico 87185

Dept. of Radiation and Surface Physics Research	**$250,000**

124. Reaction Kinetics Over Single Crystal Catalysts
D.W. Goodman

The goal of this research is to develop an understanding of surface catalyzed reactions at the molecular level using the full complement of modern surface analytical techniques. Of primary importance are those reactions relating to the synthesis of hydrocarbons from H_2 and CO. The experimental work includes the determination of reaction kinetics of hydrocarbon formation and rearrangement over single crystal catalysts. The work is carried out in a custom-built ultrahigh vacuum apparatus allowing both kinetic measurements and surface analysis. Recent studies have addressed the mechanism by which poisons and promoters alter catalytic activity and selectivity as well as the metal site requirements for catalytic activity. These measurements have utilized careful dosing of impurity atoms, either electronegative (e.g., S), neutral (e.g., Ag,Cu), or electropositive (e.g., K), onto a catalytically active single crystal substrate (e.g., Ni,Ru,Rh). These studies have established a relationship between the electronic nature of the impurity atom and its ability to alter the catalytic activity of the substrate for certain reactions. These reactions include CO and CO_2 methanation, alkane hydrogenolysis, and olefin hydrogenation. [1.6 FTE]

Surface Chemistry and Analysis Division	**$100,000**

125. FTIR Catalyst Studies
D.M. Haaland

Fourier transform infrared spectroscopy (FT-IR) is being used to study surface catalyzed reactions over supported metal catalysts. In particular, the reaction of hydrogen and carbon monoxide to form methane and higher hydrocarbons is of interest. Infrared spectroscopy allows the reactant molecules on the surface to be used as effective probes of the local environment to determine modifier-adsorbate, adsorbate-adsorbate and metal-adsorbate interactions. Therefore, FT-IR can be used to investigate the role of modifiers (promoters and poisons) on both the adsorbed reactants and the kinetics of their reaction to form methane and higher hydrocarbons. The presence or absence of long-range interactions between modifiers and adsorbants will be determined. In addition, FT-IR coupled with temperature programmed desorption and temperature programmed reaction will be used to measure relative strengths of adsorption, rates of reaction, and reaction products formed on catalysts both with and without surface modifiers. [0.8 FTE]

Solar Energy Research Institute
Golden, Colorado 80401

Division of Research	**$156,000**

126. Basic Research in Synthesis and Catalysis
J.C. Smart, D.L. Dubois, C.J. Curtis

This basic research program involves the synthesis, characterization, and reaction studies of transition metal coordination complexes and organometallic compounds for the photoconversion of N_2, CO, CO_2, H_2O, and related substrates to fuels and chemicals. It includes structural, spectroscopic, and mechanistic studies with the goal of understanding the interrelationship of molecular geometry, electronic structure, and catalytic reactivity in photochemical and photoelectrochemical transformations. Designed organometallic synthesis has yielded new bi- and trimetallic complexes with bridging fulvalene, *s*- and *as*-indacene, and trindene ligands of Ti, Zr, Ta, Mo, and Mn. Spectroscopic and photochemical studies of Co and Ni metallofulvalene and metalloindacene complexes is contributing to an understanding of their electronic structures and the potential utility of their low-lying excited states in photocatalysis. Photoelectrochemical N_2-fixation studies involve the synthesis and characterization of surface bound polymer-pendant phosphine molybdenum(O) dinitrogen complexes using combined FT-IR and electrochemical techniques. [1.5 FTE]

Separation and Analysis

Ames Laboratory
Ames, Iowa 50011

Processes and Techniques	**$1,030,000**

127. Hydrometallurgical Processing
R.G. Bautista

The development and understanding of hydrometallurgical methods of recovering metals to include: (1) dissolution (leaching); (2) separation and concentration (ion exchange, solvent extraction, and membrane separation); and (3) metal reduction from solutions (cementation, precipitation, and electrolysis) based on the equilibria, mechanisms, kinetics, and transport properties of the chemical reaction system are the related activities which are the principal objectives of this research program. The research projects presently being completed include: (1) the prediction of the concentration changes of the various species in solution during the dissolution of pyrrhotite and pentlandite by ferric sulfate and sulfuric acid; (2) the characterization of the solvent extraction mechanism of gallium in the system $GaCl_3$-$AlCl_3$-HCl-H_2O-tributyl phosphate; and (3) the electrochemical dissolution of chalcopyrite carried out in a liquid fluidized bed electrochemical reactor as as means of separating the copper, iron, and sulfur by a series of oxidation/reduction reactions. [2.0 FTE]

128. Analytical Spectroscopy
V.A. Fassel

This effort is devoted to the systematic observation of spectroscopic phenomena, with the ultimate goal of utilizing these observations for devising new spectroscopic analytical concepts that offer promise of solving singularly difficult analytical problems that either exist now or are likely to arise in the future in the various fields of energy generation (the conversion of coal to liquid and gaseous fuels, solid state materials research, and in environmental pollution). Emphasis is being placed on: (1) novel applications of electrical plasmas as vaporization-atomization-excitation-ionization sources for analytical atomic emission, mass, and fluorescence spectroscopy; (2) analytical applications of highly selective energy transfer processes from x-ray and laser beams to trace constituents in solid materials, leading to optical emission (e.g., x-ray or laser excited optical luminescence); (3) selective energy transfer from gaseous metastable species to trace level gaseous organic or inorganic constituents, with the intent to devise new analytical concepts; and (4) photoacoustic spectroscopy analytical techniques. [4.7 FTE]

129. Analytical Separations and Chemical Analysis
J.S. Fritz

A major effort is under way to improve our new method of ion chromatography, so that complex mixtures of inorganic anions and cations can be separated and analyzed with the same facility that is possible in organic chromatography. Research on ion-exchange resins is designed to provide better resins for chromatography and to give a better understanding of the important scientific problem of resin selectivity. New methods are being developed for the selective concentration of various organic compounds prior to chromatographic analysis. An improved statistical theory of chromatography has been formulated to correct some inadequacies of prevailing theories and provide a better foundation for chromatography. [2.0 FTE]

130. Mass Spectroscopy in Chemical Analysis
R.S. Houk

The general objective of this research program is to develop, evaluate, and characterize ionization techniques with potential value for analytical mass spectrometry (MS). Current efforts concentrate on improving techniques for extracting and mass analyzing ions from inductively coupled plasmas (ICPs). The value of this ion source for elemental and isotopic analysis of solutions on a rapid, direct basis is being demonstrated. Various alternate techniques for introducing samples are being studied with the ICP-MS device as an element-selective, isotopically-sensitive detector. These sample introduction methods include electrothermal furnaces or arc discharges for direct vaporization of solids and liquid chromatographic separations for determining elemental speciation via isotopic tracing experiments. Mass spectra of polar, nonvolatile organic compounds can be obtained directly from aqueous solutions provided ICP conditions are properly cooled. Temperatures, ion and electron densities, and energy transfer processes in ICP are being modeled and studied experimentally. Ionization techniques for mass spectrometric analysis of solids are also being investigated. These techniques include a laser probe for direct, absolute elemental analysis and a pulsed neutral atom beam for desorption and ionization of nonvolatile organic molecules. [2.4 FTE]

131. Lasers in Analytical Chemistry
E.S. Yeung

This program is aimed toward the development of new analytical techniques relevant to pollution monitoring, combustion diagnosis, and material evaluation in energy production. New spectroscopic concepts and instrumentation, particularly those involving lasers, are studied so that analytical methods can gain in sensitivity, selectivity, accuracy, and speed. Specific areas of concern include: (1) the development of the laser microprobe for atomic spectroscopy on surfaces; (2) new optical detectors for liquid chromatography suitable for complex organic samples; (3) nonlinear Raman methods and two-photon methods applied to analytical problems; (4) photoacoustic and interferometric concepts for improved absorption measurements; and (5) laser-induced chemiluminescence for specific gas analysis. Investigations include the fundamental principles behind the measurements, the evaluation of the analytical potentials, and the demonstration of the analytical method in representative samples. [6.0 FTE]

Argonne National Laboratory
Argonne, Illinois 60439

Division of Chemistry **$1,330,000**

132. Separations Science Related to Nuclear and Hydrometallurgical Technology
E.P. Horwitz, P.R. Danesi, H. Diamond, D. Kalina, L. Kaplan

This program has as its objectives the development of new separation processes and energy-efficient techniques applicable to nuclear and hydrometallurgical technologies and the elucidation of the basic chemistry involved. Major areas of investigation are: (1) the synthesis and characterization of new extractants for metal ion separation by liquid-liquid extraction (LLE) and supported liquid membranes (SLM); (2) the basic physical chemistry of supported liquid membranes, with emphasis on the various factors which influence the permeability rates of metal ions; and (3) the evaluation of the separation potential of new extractant and SLM systems, with emphasis on developing new methods for by-product recovery from radioactive waste, energy-efficient techniques for the recovery of critical and strategic materials from low-grade domestic sources, and new methods for processing radioactive waste streams. [8.0 FTE]

133. Study of Atmospheric Trace Gases By Mass Spectrometry
C. Stevens

The carbon isotopic compositions of atmospheric methane and natural and anthropogenic sources of methane are being measured to establish the relative distribution of these sources. In addition, we are collaborating with Dr. R. Rasmussen of the Oregon Graduate Center in analyzing the isotopic composition of methane in old air samples collected in both hemispheres since 1978. Changes in the composition reflect changes in the fluxes of enriched or depleted ^{13}C-methane. The purpose of these measurements is to provide clues for causes of an increasing concentration of atmospheric methane, whether it is caused by increasing source fluxes or a decreasing rate of removal from the atmosphere. The results of this study bear on the extent of the methane contribution to the so-called greenhouse effect and its effect on future climate changes. They also provide important quantitative knowledge of anthropogenic source fluxes of CH_4 and the global concentration of atmospheric OH radicals. [1.3 FTE]

134. Separations of Coal Macerals and Other Fossil Fuels
R.E. Winans, G.R. Dyrkacz, C.A.A. Bloomquist

The major objective of the project is to develop new methods for the separation of coal macerals. This program has been able to reduce the complexity of coal science by the separation of coals into their maceral constituents using density-gradient centrifugation. Characterization of these maceral concentrates has led to a better understanding of their role in coal chemistry. More efficient methods of separation are being explored which exploit differences in surface properties. [2.7 FTE]

Brookhaven National Laboratory
Upton, New York 11973

Dept. of Applied Sciences **$300,000**

135. Specific Molecular Property Detectors For Chromatographic Analysis
J.S. Gaffney, E.J. Premuzic

This research effort is developing novel specific molecular property detectors for use in gas and liquid chromatography. Detection schemes are devised which simplify the separation analyses by increasing the detector response for the specific molecules of interest while reducing the background noise from potential interferences. Areas of application range from process monitoring to trace analysis in organic geochemistry, environmental, and biomedical investigations. The program is currently developing monitoring devices for specific hydrocarbons and hydrocarbon classes. Use of vacuum-ultra violet (130-300nm) circular dichroism (CD) is under investigation as a means of monitoring optically active hydrocarbons eluting from a gas chromatograph (GC). This GC/CD system is using the National Synchrotron Light Source (NSLS) U9A Beamline. The spectral and thermal properties of ozone-chemiluminescence as a means of monitoring hydrocarbon classes (e.g., reduced sulfur compounds, olefins, and so forth), as well as photothermal laser spectroscopies, are also being investigated as selective and sensitive devices for chromatographic detection. [1.8 FTE]

136. Cyclic Separations Process Research
F.B. Hill

The purposes of this program are to obtain an understanding of the characteristics and basis of operation of cyclic separation processes as a class and to explore the feasibility of using these processes to perform specific separations important in the energy field. The cyclic processes of interest include pressure and temperature swing adsorption, parametric pumping, cycling zone adsorption, and various forms of preparative chromatography. Applications presently under study involve hydrogen isotope separations of concern in fusion reactor fuel processing and in heavy water reactor technology, and helium extraction from natural gas. Future work will include applications such as hydrogen recovery and purification and ion exchange separations useful in radwaste applications. Elements of the program include development of the theory of cyclic processes, measurements of equilibrium and kinetic properties of selected fluid-solid separation systems, measurement of the characteristics of cyclic separation processes employing these systems, and process design and evaluations studies. [1.2 FTE]

Dept. of Chemistry **$200,000**

137. Applications of Nuclear Methods to Analysis
G. Harbottle, E.V. Sayre, R.W. Stoenner

This program is concerned with the extension and improvement of nuclear methods of elemental analysis, particularly methods that permit the determination of many components (including trace impurities) quickly and efficiently, and with the development of computer-based multivariate statistical analysis which will permit the efficient and effective analysis of large assemblages of such analytical data. These methods are being applied to a wide variety of materials for which geographic origins are of significant interest. The effects of geochemical processes on trace element patterns are being investigated in several natural materials and artifacts made from them. Studies of the accuracy and precision of standardization in activation analysis are an important part of the project. The improved proportional counter method for carbon-14 measurement in samples as small as 10 mg is being applied to marine sediments in an attempt to account for the carbon dioxide inventory of the world. [2.7 FTE]

Dept. of Physics **$350,000**

138. Analytical Techniques With Synchrotron Radiation and Ion Beams
K.W. Jones, H.W. Kraner, B.M. Gordon

This program develops new analytical techniques for elemental analysis using synchrotron radiation from the National Synchrotron Light Source. Equipment is being designed and fabricated to produce a focused x-ray beam with a spatial resolution in the neighborhood of 10 micrometers. Techniques for precise trace element measurements with minimum detectable limits approaching 10^{-9} g/g are being developed concurrently for both bulk and microanalysis. A searching test of the new methods is made by comparison of the results obtained with synchrotron radiation with those obtained by other methods. These tests require the application of the techniques to samples obtained from a variety of energy-related fields. The use of synchrotron radiation for elemental identification is supported by the use of nuclear ion-beam analysis, which makes available complementary analytical techniques that are used to corroborate and extend the synchrotron radiation results. [4.0 FTE]

EG&G Idaho, Inc.
Idaho Falls, Idaho 83401

Idaho National Engineering Laboratory **$120,000**

139. Negative Ionization Mass Spectrometry
J.E. Delmore

This program is studying two ionization processes for application to negative ion mass spectrometry: negative surface ionization and electron capture. Surface ionization studies are focused on systems where the species of interest is chemisorbed on a low work function surface, followed by thermal desorption. To date, ions studied by this method include Cl^-, Br^-, I^-, BO_2^-, CN^-, CNO^-, and H^-. Ionization efficiency has been increased by several orders of magnitude using this technique. A unique electron capture ion source using crossed electric/magnetic fields has been theoretically modeled, designed, constructed and tested. This ion source forces electrons into a cycloidal orbit to reduce the kinetic energy to thermal values. The thermalized electrons are readily captured by gas molecules to form negative ions, without the high pressure system otherwise required for electron capture mass spectrometry. Refinement of both the experimental model and instrumentation is the major thrust of the program for the next year. [1.0 FTE]

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Physics Division **$177,000**

140. The Formation and Properties of Complexes of Helium and Hydrogen Isotopes
R.D. Taylor

The conditions for formation and the properties of a metastable, bound-state complex of ^3He and tritium are under study. T_2 decays with a half life of 12.3 years, ultimately producing a pair of ^3He atoms. However, vapor pressure time measurements show that the ^3He formed in liquid T_2 is retained in the liquid in an amount far exceeding the ordinary solubility. This complex, once formed, is found to be unstable in the gas phase, but it is virtually stable in liquid or in solid tritium. Preliminary data for solid T_2 at 20.0 K suggest that the newly formed ^3He is also bound. The electrical conductivity of solid T_2 containing the complex shows an initial decline of about a factor of three from the conductivity of the liquid. After a few days, this conductivity is about 100 times less. A new cell has been built that will allow pressure buildup measurements of liquid or solid T_2 without the complication of gas phase corrections. Other time-temperature measurements to characterize the complex include magnetic susceptibility and compositional studies of successive portions of gas removed from the cold cell. [1.3 FTE]

Monsanto Research Corporation
Miamisburg, Ohio 45342

MRC-Mound **$775,000**

141. Isotope Separation Research and Development
W.M. Rutherford, B.E. Jepson, E.D. Michaels, W.R. Wilkes

This program is concerned with the investigation of chemical exchange and liquid phase thermal diffusion as techniques for stable isotope separation. The chemical exchange work is directed toward finding significant equilibrium isotope effects in metal isotope exchange reactions with an emphasis on macrocyclic complexants and toward the development of two-phase isotope exchange processes for practical separations. The liquid thermal diffusion work is directed, in part, toward developing a basic understanding of the behavior of liquid phase thermal diffusion columns and, in part, toward gaining and interpreting experimental information about the isotopic thermal diffusion factor in the liquid phase. [3.6 FTE]

142. Atomic and Molecular Properties and Their Relationships to Separation Processes
W.L. Taylor, G.T. McConville, R.W. York

The objective of this research is to investigate the physical properties of isotopes and their mixtures. To obtain a more complete understanding of gaseous mixtures of hydrogen isotopes, in particular, the mechanisms for isotopic exchange in such mixtures, measurements of the formation of DT in mixtures of $D_2 \cdot T_2$ are being made as a function of pressure, initial T_2 concentration, and temperature. The interaction with D_2 is very complex, and the presence of excited state molecules plays a definite part in the reaction. Such information will be useful in design criteria for fuel handling systems in the controlled-thermonuclear power program. Total cross sections are being measured for the permanent gases with supersonic molecular beams. The data are analyzed to yield the fundamental interactions of the colliding species. The temperature range of diffusion measurements in binary gas mixtures is being extended to ~2500°C by means of a Ta/W diffusion cell operating in a vacuum furnace. The thermodynamics of the thermal diffusion process is under study in a "swing separator" instrumented with thermistors fo*in situ* and real time analysis of the separation process. Ortho- and para-deuterium are being separated in a cryogenic adsorption column and will be made available to the Stable Isotope Inventory Program. [4.2 FTE]

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Analytical Chemistry Division **$1,352,000**

143. R&D in Secondary Ion Mass Spectrometry
W.H. Christie, R.E. Eby, P.J. Todd

A rapid growth has occurred in recent years in particle sputtering as a means for producing atoms and ions for mass spectral analysis. More recently it has been observed that secondary ion mass spectometry (SIMS) offers a means of studying organic as well as inorganic materials. The major thrust of our research program has shifted in this direction, and our approach to organic SIMS has been to interface an in-house developed secondary ion source with a tandem three-sector mass spectrometer. This combination will be used to investigate the chemistry and physics of secondary ion emission from both volatile and involatile organic species. In inorganic SIMS, we plan to investigate laser induced resonance ionization of sputtered neutrals using a recently acquired microbeam instrument that is now being modified for these studies. Fundamental information concerning the sputtering process will be obtained since resonance ionization allows one to probe the excited electronic states of neutral atoms ejected during a sputtering event. This information will be used to refine the theory of sputtering phenomena including secondary ion emission which is the basis for SIMS. [2.0 FTE]

144. Mass Spectrometry R&D For Organic Analyses

G.L. Glish, P.J. Todd, E.H. McBay, S.A. McLuckey

This task consists of studies in two general areas of organic mass spectrometry. Both are experiencing rapid growth in popularity as analytical techniques even though much is yet to be understood about the underlying chemical and physical principles. These areas are: (1) mass spectrometry/mass spectrometry (MS/MS); and (2) desorption ionization (DI). The main thrust of this task is to investigate the chemical and physical phenomena associated with these areas to further the understanding and therefore make the application of MS/MS and DI easier for the general mass spectrometrist. The studies of these areas are in many ways complementary. MS/MS is a very good tool to study gas phase ionic structures and thus can be used to help elucidate chemical processes which occur during DI. Conversely, DI can be used to generate unique types of ions which can be used to assist in extending the understanding of MS/MS. Of particular interest is the gas phase ion chemistry and physics involved in MS/MS. Studies in these areas will not only better the understanding of the basic phenomena in MS/MS, but also the basic processes in mass spectrometry in general. [2.2 FTE]

145. Advanced Spectroscopic Methods For Chemical Analysis

L.D. Hulett, J.M. Dale, T.M. Rosseel

The objective of this research is to explore new physical phenomena for applications as spectroscopic methods. Positron spectroscopy is being evaluated for characterization of surfaces and bulk materials, doing chemical analyses, surface area measurements, and solid state defect studies; the monoenergetic positron sources developed earlier in this project and the ordinary fast sources are being used. Ions from the EN Tandem Accelerator and the Holifield Heavy Ion Facility are being used to induce heavy ion x-ray satellite emission spectra (HIXSE) for studies of valence states of metal alloys and other materials. X-ray diffraction and electron microscopy are being applied to special analytical problems dealing with laser research. The positron and heavy ion methods are being developed for use in other programs, such as surface modification, the High Temperature Materials Laboratory (HTML), and mass spectroscopy research. Other groups at State University of New York, Fredonia, Duke University, and the University of Missouri are also collaborating with this program. [2.8 FTE]

146. Research Development and Demonstration of Advanced Chemical Measurement Techniques

H.H. Ross, J.M. Ramsey, L.N. Klatt, W.B. Whitten, J.P. Young

New spectroscopic and instrumentation techniques are being developed that have the potential of meeting critical measurement needs in the analytical community. A new project that employs lasers and phase conjugate optics may lead to a whole new concept in laser scanning systems. Time resolved fluorescence spectroscopy is being developed for a broad range of important analytical applications. Fourier transform microwave spectroscopy is being pushed for the rapid quantitation of complex organic and inorganic mixtures. A new computer system is being programmed to collect data for this project as well as carry out the fast Fourier transform processing that is needed. Ongoing studies of laser excited optogalvanic spectroscopy will be extended to diagnostic studies of plasmas used in chemical vapor deposition experiments. We are starting a new research program that exploits robotics in analytical chemistry. [3.8 FTE]

147. Mass Spectrometric R&D For Inorganic Analyses

R.L. Walker, H.S. McKown, D.H. Smith, D.L. Donohue, D.E. Goeringer

The objective of this research is to improve isotopic ratio mass spectrometry and to extend its areas of application. Areas in which improvement is being sought include instrumentation and methodology, precision of analysis, and elemental specificity. Our laboratory houses state-of-the-art, high sensitivity, multistaged mass spectrometers to provide high quality isotopic ratio measurements on extremely small samples (~1 ng). Low-level separations techniques are carried out in a Class 100 clean room and isotope dilution is used extensively for quantitation. Resonance ionization mass spectrometry has been applied successfully to uranium and plutonium. Sensitivity and precision are quite good (10 ng samples, 0.5% standard deviation). Spectral characterization of six elements (Pu, U, Th, Cm, Np, Am) was carried out in the 580-600 nm range. A comparison of pulsed versus continuous wave laser ionization will be carried out next. A double spike (internal standard) of plutonium has been studied using NBS SRMs; it affords an improvement in precision of a factor of five over conventional techniques. A preliminary evaluation of our channel electron multiplier array (position sensitive) detector has been completed. [2.3 FTE]

Chemical Technology Division **$1,424,000**

148. Chemical and Physical Principles in Multiphase Separations

C.H. Byers, R.M. Wham, C.D. Scott

Fundamental chemical engineering investigations include new concepts and basic understanding of multiphase separation methods. Fluidized and expanded beds are stabilized by the imposition of an electric field, thus exhibiting the desirable sorption characteristics of fixed beds, while the pressure drop is approximately half the fixed bed. The applicability of this principle to a novel method for moving bed sorption is under study. Mass transfer enhancement in dispersed-phase systems by forcing the oscillation of small droplets in a continuous medium is being investigated. Preliminary results show that droplet motion can be forced by an oscillating electric field. A study to investigate separation phenomena associated with the distribution of a solute between a liquid and solidified (frozen) solvent has been initiated. Preliminary results indicate that chromatographic separation of selected solutes is possible. [5.3 FTE]

149. Chemical Separations For Tritium

P.W. Fisher

This program studies fundamentals of tritium separation techniques needed for fusion and fission reactor systems. Recent studies have been concerned with tritium sorption from liquid lithium by metallic getters such as yttrium and yttrium alloys. Tritium diffusion rates in both solid and composite metals were investigated, and a correlation was developed which describes the behavior of composites. More recent studies have been directed at the interactions of tritium and tritiated water molecules at solid surfaces. These studies will investigate the roles of sorption, exchange reaction, desorption, and bulk diffusion processes on tritium uptake and release from surfaces. More fundamental understanding of these phenomena will be useful to a number of problems in fusion and fission reactor systems, such as contamination of surfaces, retention of tritium following accidental releases, exchange of molecular tritium with the more hazardous oxide, and decontamination of used components. [1.4 FTE]

150. The Chemistry of Solvation Applied to Separations

J.E. Mrochek, H.D. Cochran

Solvent-solute interactions (solvation) in both ionic and nonionic media are of paramount importance to the understanding of many separation methods. This program investigates, in a systematic and fundamental manner, both short- and long-range solvation effects in mixed media. Current studies are directed at selected aprotic and supercritical solvents. Spectroscopic measurements, including both ultraviolet and nuclear magnetic resonance (nmr) relation techniques, are used to study both bound (inner) and bulk (outer) solvent molecules, and the results are related to thermodynamic properties. The studies are currently focusing on inorganic chloride solutes which have not been investigated extensively in the past, but have potential important applications. The studies with aprotic media are directed at speciation of complexes and modifications caused by introduction of known quantities of water into the systems. Studies under supercritical conditions are attempting to relate the heretofore empirical binary interaction parameter to an intermolecular potential function (e.g., Lennard-Jones potential). Subsequent studies will investigate polar solvents where the Stockmayer potential is appropriate. The results of these studies will increase our understanding of solute-solvent interactions, improve our predictive capabilities, and eventually be useful to a number of separation processes. [3.7 FTE]

151. Chemistry of Actinides and Fission Products

L.M. Toth, D.J. Pruett

The chemistry of actinides and of fission products is investigated with emphasis on the properties that affect separation and partitioning in the nuclear fuel cycle. The broad scope of subjects includes: (1) photochemical studies; (2) the structures and properties of polymer materials; (3) solvent extraction and coextractions, and (4) the induction times and precipitation in pseudo stable process and waste streams. Recent studies have concentrated on the solvent extraction of heptavalent technetium and rhenium in nitric acid systems with and without uranium, and on the photochemical reduction of heptavalent technetium to the V and IV states in nitric and hydrochloric acids. New research will include the photochemistry of low temperature uranium and plutonium frozen solutions or salts and the catalytic effects of Pu(IV) on actinide redox reactions. [3.0 FTE]

Chemistry Division	**$690,000**

152. Chemical and Structural Principles in Solvent Extraction

J.H. Burns, C.F. Baes, Jr.

The purpose of this research is to obtain basic information about solvent-extraction systems that may lead to improved processes for recovery of strategic materials for national energy needs. The approach is to investigate known successful processes with the aim of understanding, on a molecular level, the mechanism by which they operate, and to determine which variables of reactivity and structure are important to their success. The structures of solvent-extraction complexes in the solid state and in solution are being studied by the methods of x-ray diffraction and nuclear magnetic resonance. Among the systems being analyzed are those involving the extraction of uranium by organophosphorus ligands and those of alkaline earths by macrocyclic ethers. The structural information obtained is being used to develop criteria for solvent extraction which will have general applicability. These criteria are being used in the design of more effective extraction reagents for the actinides and could provide a guide for the development of new techniques for the separation of other metals. [1.8 FTE]

153. Chemical Separations By Complexation Phenomena

W.J. McDowell, B.A. Moyer

Basic scientific understanding of methods for separating mixed elements, compounds, or aggregate materials is being obtained by systematic and fundamental studies of equilibria and mechanisms and of the properties of the components in selected separations systems. The present emphasis is on solvent extraction and ion exchange systems, which are well defined and of widespread concern. A major aim is understanding of the relationship between reagent structure and selectivity for particular ions or molecules, so that agents can be designed for improved selectivity, kinetics, and phase behavior. Multidentate extractants, including chelating and macrocyclic compounds, are emphasized because their known complex-forming behavior gives basis for designing specificity into reagents. Detailed studies include: (1) the effects of a range of functional groups when they are attached to carrier molecules or resin skeletons; (2) synergistic combinations of different functions; and (3) elucidation of the structures of adducts of metals with ligands that are known to be selective. [3.7 FTE]

Pacific Northwest Laboratories
Richland, Washington 99352

Dept. of Biology and Chemistry	**$140,000**

154. Fundamental Phase Partitioning in Supercritical Fluid Chromatography

R.D. Smith, B.W. Wright, H.R. Udseth

The goal of this program is a fundamental understanding of the kinetic and thermodynamic constraints upon partitioning of a solute between a supercritical fluid and a supported phase. The program involves investigation of fluid phase reactivities, solubilities, and phase partitioning kinetics relevant to supercritical fluid chromatography and extraction phenomena. Phase partitioning and related chromatographic processes are being studied using direct fluid injection-mass spectrometry, classical equilibrium sampling, and various optical techniques. The program is directed at gaining an understanding of chromatographic processes for polar amd mixed supercritical fluid and solute systems and the kinetic and thermodynamic limitations upon separations in supercritical media. Experimental results are being compared with both theoretical methods for prediction of fluid phase solubilities and actual chromatographic separations for model systems, with the aim of identifying critical parameters for the development of improved chromatographic systems. [1.0 FTE]

Dept. of Radiological Sciences **$700,000**

155. Laser-Based Analytical Techniques
B.A. Bushaw, B.D. Cannon, T.J. Whitaker

The objective of this program is to develop and evaluate ultrasensitive and highly selective laser-based analytical techniques. Photon correlation spectroscopy has been used to enhance the detection of Na, Rb, and Sr isotopes. Both photon burst and time interval distribution analysis have been used for single atom counting. The observed detection limits, 10 atoms per second crossing the laser beam or about 0.1 atom/cm^3, are governed by nonstatistical noise behavior of the photon counting electronics. Time correlation filtering of the detection of multiple photons from a single atom, combined with single frequency dye laser excitation, may provide resolution better than the natural Lorentzian lineshape. Isotopic selectivities one to two orders of magnitude better than observed in the normal fluorescence spectra have been demonstrated. Current efforts are directed toward extending these techniques to other elements and applying them to the analysis of discrete samples. A vacuum graphite furnace, similar to that used for flameless atomic absorption analysis, is to be used as an atomization source for many sample types. Other species may be observed by supersonic beam sampling of plasma discharges. Metastable states, formed in the plasma, are of particular interest for the detection of noble gases and other spectroscopically difficult elements. [1.4 FTE]

156. Analytical Mass Spectrometry Research
R.L. Gordon, J.M. Kelley, D.M. Robertson, J.J. Stoffels

This task develops new knowledge and techniques to extend the application of mass spectrometry to problems in chemical and isotopic analyses. The task: (1) elucidates physicochemical mechanisms responsible for efficient ion production in isotopic analysis by surface ionization mass spectrometry; (2) develops methods for the control of surface work function of ion sources; (3) develops techniques for application of mass spectrometry to real-time analysis; and (4) establishes new ionization techniques. Surface analytical tools are used to establish physical and chemical properties of surface ionization sources and to identify chemical pathways responsible for ion production. The direct-inlet technique for real-time mass spectrometry uses innovations in ion sources, mass separators, and ion detectors. Laser-assisted ionization is being developed for new mass spectrometry ion sources. [3.3 FTE]

157. Analytical Atomic Absorption Spectrometry Research
D.L. Styris, J.H. Kaye

This program elucidates experimentally the mechanisms that control sample vaporization in furnace atomic absorption (FAA) spectrometry. Vaporization models that are developed from these results provide understanding of chemical treatment and furnace effects, and thus establish the basis needed to help broaden and improve application of contemporary FAA spectrometric analysis. The neutral atoms, ions, and molecular species that appear in vapor phases during the temperature rise of the furnace are monitored simultaneously by atomic absorption and mass spectrometric techniques. Correlation of results from these experiments with furnace temperature and applications of chemical thermodynamic and kinetic data help to identify and characterize the controlling chemical and physical processes. Vitreous carbon, tantalum, and graphite furnace materials are being used presently in order to model the Group IIA element vaporization that occurs in presence of these furnace materials and the intragroup matrix modifiers. The experimental technique is also being used to determine spatial distributions of gaseous species within the furnaces. [1.3 FTE]

Sandia National Laboratories
Albuquerque, New Mexico 87185

Dept. of Laser R & D **$150,000**

158. Laser Based Analytical Methods
A. Owyoung, A.V. Smith, J.P. Hohimer, T.D. Raymond

This research is directed toward the development of new, highly sensitive, species-specific laser-based analytical techniques with capabilities beyond the reach of conventional methods of analysis. To this end our program emphasizes: (1) the determination of the utility and limitations of newly developed laser-based techniques (such as multiphoton ionization spectrometry, MPIS) in analytical applications; (2) the integration of such techniques with more conventional methods of analysis (such as mass spectrometry) to provide analytical capabilities of increased dimension; and (3) the exploration of entirely new laser-based concepts having potential utility for analytical applications. This year we are performing a direct comparison between laser ionization and electron beam ionization methods for TOF mass spectrometry. We are also exploring the use of laser ionization methods for rotational-vibrational spectroscopy and the use of laser sources to enhance the utility of field-ionization mass spectrometry. [1.0 FTE]

Chemical Engineering Sciences

Lawrence Berkeley Laboratory
Berkeley, California 94720

Applied Science Division **$239,000**

159. Turbulent Combustion
F. Robben, R.K. Cheng, L. Talbot

The effect of fluid mechanical turbulence on combustion is being studied experimentally for premixed fuel/air conditions in two idealized flow configurations: (1) turbulent boundary layer over a strongly heated wall where lean combustion occurs;

and (2) an unconfined v-shaped turbulent flame. Density and velocity fluctuations and several of their cross correlation parameters are measured, using techniques based on laser Rayleigh scattering and laser Doppler velocimetry. These measurements are useful to characterize the features of the flame structures and their effects on the turbulent flow field. The initiation and development of combustion in the heated boundary layer are found to be dominated by the large-scale turbulence structures. Measurements of Reynolds stress in the v-shaped flame have shown that a mean-gradient transport model for production of turbulent kinetic energy is not appropriate for these flames. [2.5 FTE]

Materials and Molecular Research Division **$146,000**

160. High-Pressure Phase Equilibria in Hydrocarbon-Water (Brine) Systems
J.M. Prausnitz

Phase equilibria are required for efficient design of large-scale separation processes (e.g., distillation and extraction) in the chemical and related industries. In this context, "efficient" refers to optimum use of raw materials and to conservation of energy. Since the variety of technologically-important fluid mixtures is extremely large, it is not possible to obtain all desired equilibria from experiment. Therefore, the objective of this research is development of molecular thermodynamics for interpretation and correlation of selected phase-equilibrium data toward reliable general prediction of phase equilibria for engineering. The correlations are expressed through semi-theoretical physico-chemical models in a form suitable for computer aided design. In this research, particular attention is given to those systems that are of primary interest in energy-related industries, especially those concerned with fossil fuels and fossil-fuel-water mixtures. Development of molecular thermodynamics calls for a combination of theoretical, computational, and experimental work. Further, it demands simultaneous awareness of progress in molecular science and of realistic requirements for engineering design. [2.1 FTE]

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Theoretical Division **$73,000**

161. Thermophysical Properties of Mixtures
J.J. Erpenbeck

Evaluation of the thermophysical properties of mixtures of particles that interact through the hard-sphere potential has been initiated, using equilibrium techniques of Monte Carlo (MC) and molecular dynamics (MD) as well as non-equilibrium molecular dynamics (NEMD). Properties investigated cover the equation of state and transport properties (including mutual diffusion, shear and bulk viscosity, and thermal conduction). A combined Monte Carlo and molecular dynamics (MCMD) calculation for the single-component hard-sphere fluid has yielded equation of state data of extremely high precision. Combining these data with the Pade' approximants to the virial series (using the known virial coefficients through B_5) we have obtained estimates for the sixth and seventh virial coefficients and approximants of sufficient precision to fit the MCMD data over the fluid regime, up to a density of 1/1.6 of close-packed. Study of the shear viscosity of the hard-sphere fluid by NEMD has shown the existence of a shear-induced phase transition to a two-dimensionally ordered phase. It also shows the viscosity coefficient to decrease regularly with increasing shear rate up to the phase transition. For isotopic (mutual) diffusion, comparisons of Green-Kubo and NEMD calculations have shown the methods to agree, yielding a mutual diffusion constant roughly 13% greater than the prediction of the Enskog theory, for a volume three-times close-packing. The enhanced diffusion appears to arise from the existence of a long-time (perhaps $t^{-1/2}$) tail in the velocity-velocity time correlation function. [0.5 FTE]

National Institute for Petroleum and Energy Research (NIPER)
Bartlesville, Oklahoma 74005

Processing and Thermodynamics **$177,000**

162. Thermodynamic Characterization of Condensed-Ring Compounds
B.E. Gammon

Research continues on synthesis, purification, and measurement of thermodynamic properties of polycyclic aromatic hydrocarbons and their hydrogenation products and for similar polycyclic, organic, nitrogen compounds. These substances are important in processing of coal, oil shale, and heavy petroleum to produce liquid fuels and chemical feedstocks. Preparation of manuscripts is in progress reporting thermodynamic properties of 2,2'-dimethylbiphenyl, isoquinoline, quinoline, and 4-methylphenanthrene. Measurements are nearing completion on acridine and phenanthridine; several other compounds are purified awaiting measurements. Synthesis and purification of others are in progress. Derived Gibbs energies of formation facilitate an understanding of hydrocracking and denitrogenation. The data also form the base for improved correlations based on molecular structure. The comprehensive experimental program involves enthalpy of combustion, low-temperature adiabatic calorimetry (third-law entropy determinations), vapor pressure manometry, and Raman and infrared spectroscopy with molecular statistical mechanics. [3.0 FTE]

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Chemical Technology Division **$99,000**

163. Fundamental Processes in Sorption Pumping and Transfer Operations Using Deep Beds of Sorbents
C.H. Byers, J.J. Perona

A fundamental framework for predicting the performance of deep-bed sorption systems is being developed for application to processes involving pumping, transfer, and storage of materials by sorption on deep beds of sorbents. Currently such techniques are utilized in a number of energy production and storage applications. An experimental program is in progress to determine the relative significance of heat and mass transfer, pressure drop, sorption equilibrium, and reaction kinetics. In the current phase, sorption processes at cryogenic temperatures in the molecular flow regime are controlled by mass transfer resistance. The assumptions used in an analytical solution to the problem are under experimental investigation in a recently reworked and expanded experimental system. Simultaneous numerical solutions are under development. [1.1 FTE]

Sandia National Laboratories
Livermore, California 94550

Combustion Technology Dept. **$229,000**

164. Analysis of Reacting, Turbulent Flows
W. Ashurst, P. Barr, B. Sanders

This research focuses on understanding the detailed mechanisms of heat, mass, and momentum transfer in the mixing region of reacting shear flows. Activity involves development of an unsteady turbulence computational procedure for application to flows with high Reynolds numbers and large heat release. The vortex dynamics simulation procedure will be used to study the transport of a conserved scalar in both homogeneous and inhomogeneous turbulent flows in two and three space dimensions. This procedure is unique in that it relaxes some of the restrictive assumptions employed in most conventional turbulence models, and the method is capable of resolving the time-dependent coherent structures that have a first order influence on the transport of chemical species. A hybrid computational scheme will be constructed using the Lagrangian vortex dynamics procedure for small-scale turbulent structures, and the Eulerian large-eddy simulation procedure for large-scale structures. This hybrid method shows promise for a major breakthrough in turbulence modeling, as the time dependent flowfield can be described over a wide range of length scales important to combustion. [1.5 FTE]

OFFSITE INSTITUTIONS

Heavy Element Chemistry

Florida State University
Tallahassee, Florida 32306

165. ***Research in Actinide Chemistry***
G.R. Choppin, Dept. of Chemistry **$95,700**

This research is concerned primarily with complexes of actinide elements in aqueous solution. To supplement data on trivalent actinides, similar systems are investigated for trivalent lanthanides using the wider variety of techniques available with the latter elements. Our studies include measurements of the thermodynamic parameters of complexation of both inorganic and organic ligands, of the kinetics of complexation, of the spectroscopic properties of complexed species using electronic (f-f) transitions and nuclear magnetic resonance and of the redox properties of the actinides. Our interest is focused on the fundamental aspects of the factors that determine the nature and extent of formation of actinide complexes. The ligand studies have potential interest in separation schemes of the actinides or in their environmental or biological behavior. It is hoped that these studies will lead to the development of useful models for the behavior of actinide ions in a variety of natural solution systems.

SRI International
Menlo Park, California 94025

166. ***Chemistry of Gaseous Lower-Valent Actinide Halides***
D.L. Hildenbrand, Physical Sciences Division **$88,400**

The objective of this program is to provide accurate thermochemical information for key actinide halide, oxyhalide, and related systems, starting with uranium halides, so that the basic factors underlying the chemical bonding and chemical reactivity in these systems can be elucidated in a systematic way. Our principal focus is on the gaseous halides, mainly the lower-valent halides, since there is little or no thermodynamic or spectroscopic information on these species. Bond dissociation energy and absolute entropy data are derived from chemical equilibrium measurements made primarily by high temperature mass spectrometry. The bond dissociation energies and their variation with the number of halogen ligands yield insight into the electronic character of the bonding, while the absolute entropies provide useful checks on assigned structures and electronic partition functions. Current studies are concerned with the U-Br, Th-F, and Th-Cl systems; all of the lower-valent halides in these systems have now been generated from effusive sources, identified by mass spectrometry, and thermochemically characterized. A clear pattern of bond dissociation energies is beginning to emerge; this pattern will be useful in modeling the thermochemistry of the heavier actinide halides, which will be much more difficult to study.

University of New Mexico
Albuquerque, New Mexico 87131

167. ***Development of Surface Immobilized Ligands For Actinide Separations***
R.T. Paine, Dept. of Chemistry **$73,000**

The general objectives of this program are to develop systematic synthetic methods for the attachment of extractants to solid supports and to screen the immobilized extractants as selective ion chromatography materials for the separations of metal ions present in nuclear fuel reprocessing and industrial waste solutions. Within this project fundamental investigations of steric and electronic effects which influence and modify extractant-metal ion interactions are in progress. Isolated liquid-liquid extraction complexes are studied at the molecular level by spectroscopic and x-ray crystallographic methods. The resulting molecular architecture data are used to design improved extractants and to model surface immobilized extractant-metal interactions. Extraction equilibria for several phosphonate extractants attached to polymer backbones and silica in contact with lanthanide and actinide ions are being obtained.

University of Tennessee
Knoxville, Tennessee 37996-1200

168. ***Magnetic Measurements of the Transuranium Elements and Characterization of Actinides in Primary Waste Forms***
P.G. Huray, Dept. of Physics **$100,000**

A SQUID based micromagnetic susceptometer in the facilities at the Transuranium Research Laboratory is being used to measure the magnetic properties of americium, curium, berkelium, californium, and einsteinium metals and compounds. The research catalogues magnetic behavior of unmeasured heavy actinides between 4.2 K and room temperature and 0 to 5 tesla. The study provides a measure of the degree of localization of the 5f electrons, and examines the effects produced by neighbor-neighbor overlap. The effective magnetic moments of heavy atoms and the observed magnetic transition temperatures (if any) are examined within the context of the intermediate coupling model. Current work deals with the saturated moments of dhcp californium-249 metal and the degree of magnetic order attained in the limit of low temperatures and high fields. A practical result of the work is the identification of electronic configurations of transuranium elements in primary nuclear waste forms.

169. ***Physical-Chemical Studies of the Transuranium Elements***
J.R. Peterson, Dept. of Chemistry **$135,000**

This program provides training for pre- and postdoctoral students in chemical research with the transuranium elements through continuing investigations of the basic chemical and physical properties of this group of elements and the interpretation and correlation of the results obtained. New knowledge is being accumulated for the following areas: (1) the role of the 5f electrons in the bonding in actinide elements and compounds; (2) the relationships of metallic structures to metallic valence and radius; (3) the extent and magnitude of the actinide contraction; (4) the magnetic, thermodynamic, spectroscopic, and crystallographic properties of these materials as related to general theories; (5) the effect of self-irradiation on chemical and physical properties; (6) the chemical and physical consequences of radioactive decay in the bulk-phase solid state; and (7) in general, the range of validity of the actinide hypothesis. Research activities include: (1) spectroelectrochemical studies in aqueous and nonaqueous media; (2) measurement of heats of solution; (3) absorption and Raman spectroscopies in solution and solid state (the latter as a function of temperature or pressure); (4) structural changes as a function of temperature or pressure; (5) direct or indirect (via radioactive decay) synthesis of compounds containing unusual oxidation states; (6) determination of the structures of einsteinium compounds; amd (7) studies of the fundamental chemistries of the transeinsteinium elements.

Photochemical and Radiation Sciences

Alabama A & M University
Normal, Alabama 35762

170. *Photoacoustic/Laser Spectroscopy of Halogens and Mixed Halogens For Energy Purposes*
P. Venkateswarlu, Dept. of Physics **$100,000 (24 mo.)**

The photoacoustic spectrometer for the study of the energy level structure of the halogen molecules is being set-up. A nitrogen/dye laser system is used as the excitation source. The acoustic signals are detected with microphones. The signal processing is done by a boxcar integrator. The various components (e.g., photomultiplier and microphone detectors, amplifiers, and other optical elements) are being procured. A quartz absorption cell is also being fabricated.

Boston University
Boston, Massachusetts 02215

171. *Investigation of the Triplet States of Chlorophylls*
R.H. Clarke, Dept. of Chemistry **$173,300 (24 mo.)**

The characterization of the structures assumed by chlorophyll molecules upon aggregation in photosynthetic systems is important for an understanding of the mechanisms of energy conversion in photosynthesis. Since the properties of the excited triplet state of the pigment molecules such as the electron distribution and excited state dynamics are sensitive to the surrounding interactions and to the state of aggregation, triplet state properties serve as a convenient and nondestructive probe into the makeup of photosynthetic systems. Our present research project uses optical detection of magnetic resonance spectroscopy and raman spectroscopy to investigate the triplet state properties of the chlorophyll molecule in lipid bilayers, in protein matrices, and as films deposited on surfaces. These measurements allow an evaluation of *in vitro* chlorophyll systems for structural features proposed as models for the antenna and reaction center of naturally occuring photosynthetic systems and for their general applicability as model systems for photosynthesis.

172. *Study of Intermediates From Transition Metal Excited-State Electron-Transfer Reactions*
M.Z. Hoffman, Dept. of Chemistry **$75,000**

This research is concerned with the kinetic and mechanistic behavior of intermediates that result from excited-state electron-transfer reactions involving transition metal coordination complexes, quenchers, and sacrificial electron donors in solution. These intermediates are generated by means of continuous and flash photolysis, and from the interaction of substrates with radiation-generated radicals using continuous and pulse radiolysis techniques. The emphasis of the work is currently on the modes of formation and decay of reduced viologens. Viologens form photoactive charge-transfer complexes with sacrificial electron donors; the magnitude of complexation, photoreduction, and luminescence is being studied as a function of pH and solution composition. Ion-pairing and complexation have a significant effect on the quantum yield of reduced viologen when the system is photosensitized by ruthenium(II)-polypyridyl complexes. Viologens are reduced by EDTA radicals; hydrogenation of reduced viologens is minimized, and the yield of hydrogen is maximized, upon interaction of reduced viologens with catalytic platinum in the presence of EDTA. The goal of the research is to understand the fundamental chemistry governing the generation of energy-rich charge-separated species.

173. *Formation of Fuel via Photochemical Electron Transfer*
G. Jones, Dept. of Chemistry **$192,000 (24 mo.)**

This research involves investigation of photochemical electron transfer reactions which are of potential utility in photoformation of fuel or useful chemicals. New reagents are under development that would permit the separation of oxidation and reduction components through temporary storage of redox equivalents in stable photoproducts. Novel sulfur heterocycles capable of two-electron oxidation are of particular interest, as electron relays for experiments involving electron transfer in solution. Studies also encompass photoinduced electron transfer reactons of organic dyes which are bound to water soluble polymers. Applications of electron transfer in photochemical decomposition of hydrogen sulfide, hydrogen halide, as well as water are under consideration.

Brandeis University
Waltham, Massachusetts 02254

174. *Photochemical Reactions of Complex Molecules in Condensed Phase*
H. Linschitz, Dept. of Chemistry **$95,000**

The purpose of this project is the identification and evaluation of factors governing the efficiency of primary radical formation in photochemical redox reactions. This is a general problem in photochemical energy conversion since charge-transfer kinetic intermediates may lead either to radical products or dissipative quenching. Reaction rates and quantum yields are measured by laser flash photolysis on redox systems including particularly porphyrins or aryl ketones, with inorganic anions or water itself as donors. The major phenomena to be understood are the mechanism of the direct photoxidation of water by ketone triplets and the sharp increase in radical yield at high anion concentrations. Studies on covalently linked porphyrin-quinone systems are in progress, to determine effects of donor-acceptor distance, orientation, and dielectric medium. Spectroscopic and photochemical properties of porphyrin dimers are being studied, as models for photosynthetic reaction centers. Other research is concerned with photo-isomerization of dipyrryl-methenes and shifts in proton-transfer equilibria accompanying formation of rotational conformers.

Brown University
Providence, Rhode Island 02912

175. A Unified Approach to Characterization of Collisions Between Reactive Radical Pairs in Solution
R.G. Lawler, Dept. of Chemistry **$75,000**

A project is under way to systematically characterize the reactive and unreactive encounters between simple organic and inorganic free radicals in aqueous and organic solvents by comparing the kinetics of bimolecular radical decay as measured by EPR with concurrent measurements of bimolecular contributions, especially Heisenberg spin exchange, to electron relaxation times. Radicals are generated at present primarily by pulse electron radiolysis of aqueous solutions of simple inorganic ions or organic acids and alcohols using facilities at Argonne National Laboratory. Studies are being extended to organic solvents using peroxides as radical precursors and employing EPR detected photolysis. Theoretical models are being developed both to extract data from rapidly varying magnetic resonance spectra detected by pulsed methods and to interpret the ratio of reaction to exchange probabilities in terms of molecular properties of the radicals and the medium in which they react.

Carnegie-Mellon University
Pittsburgh, Pennsylvania 15213

176. Solar Energy Conversion in Homogeneous Solution
R.M. Richman, Dept. of Chemistry **$50,000**
(9 mo.)

The goal of this project is to study the photochemistry of compounds that are likely to photodisproportionate. This mechanism has the potential for doing useful oxidations and reductions without the need for a nondissociative long-lived charge transfer excited state. Irradiation of μ-oxo-bis((tetraphenylporphinato)-iron(III)) at $\lambda \geq 440$ nm yields the ferryl ion, FeOTPP. Irradiation with sunlight of a cyclohexene solution results in catalytic oxidation to cyclohexene-1-one with several thousand turnovers. Inclusion of thallium (III) benzoate may yield the epoxide. Flash photolysis allows direct observation of the transient FeOTPP. Analogous photochemistry is observed with $(FeTPP)_2N$ and $(FeTPP)_2C$. Use of charged porphyrins allows study in aqueous solution, but the quantum yield at 410 nm is still $\sim 10^{-4}$. Irradiation in the presence of CoTPP may yield the novel mixed-metal FeTPP-O-CoTPP. Irradiation of $[Ru(NH_3)_5]_2O^{4+}$ results in substitution followed by reduction.

Charles F. Kettering Research Laboratory
Yellow Springs, Ohio 45387

177. Particulate Models of Photosynthesis
G.R. Seely. **$67,900**

The program consists of the investigation of photophysical and photochemical properties of chlorophyll, absorbed together with other amphiphilic molecules on particles of polyethylene swollen with low molecular weight hydrocarbon diluents. When suspended in aqueous media, the particles are intended to provide a viscous medium for anchorage of the hydrophobic parts of amphiphilic molecules. In general, chlorophyll is maintained in monomeric form in the presence of amphiphiles that interact with it, such as alkylamides, or as fluorescent dimers or higher aggregates at greater concentration. Specific aspects under investigation include absorption, fluorescence, and CD spectroscopy, energy transfer among chlorophyll species, and photochemistry. With regard to the last the behavior of particles with chlorophyll and oxidizing amphiphilic ligands is receiving particular attention.

Clarkson College of Technology
Potsdam, New York 13676

178. Photochemical Solar Energy Conversion in Surfactant Vesicles
J.H. Fendler, Dept. of Chemistry **$155,000**
(24 mo.)

Utilization of surfactant vesicles for solar energy conversion continues to be the goal of this project. The main thrust of our research has centered upon the use of vesicles and polymerized vesicles for the *in situ* generation of catalyst coated colloidal semiconductors and upon their employment in efficient solar hydrogen generation. Compartmentalization of appropriate precursors in controlled concentrations has led to the reproducible formation of small catalyst coated uniform semiconductors in the vesicles. Additionally, subsequent to band-gap excitation, undesirable electron hole back recombination has been observed to diminish in the unique microenvironments provided by the vesicles. Efficient photosensitized hydrogen generation has been demonstrated on using *in situ* generated platinum coated CdS colloidal semiconductors in vesicles. Thiophenol has been used as a sacrificial electron donor. Current research is directed toward the optimization of these and related systems.

Clemson University
Clemson, South Carolina 29631

179. Intramolecular Energy Transfer Reactions As a Method For Metal Complex Assisted Production of Hydrogen
J.D. Petersen, Dept. of Chemistry **$135,500**
(24 mo.)

The current research effort concentrates on coupling highly absorbing metal centers to potentially photoactive metal centers (e.g., metal dihydrides) by covalent bonding through bridging ligands. This is done in order to use low energy light to drive useful chemical reactions by intramolecular energy transfer processes. Major emphasis has been on bridging ligands that will chelate both metal centers such as 2,2'-bipyrimidine and 2,2'-biimidazolate, and form short, highly-conjugated links

$[Ru(bpym)Cl_2]_2(bpym)$, which is black in color and has two potential derivative sites on each metal center.

Columbia University
New York, New York 10027

180. Laser Enhanced Chemical Reaction Studies
G.W. Flynn, Dept. of Chemistry **$90,000**

This project is aimed at the study of chemical reactions of laser pumped molecules, with particular emphasis on the role of vibrational energy transfer processes in chemical dynamics. Fast hydrogen, chlorine, and deuterium atoms are being produced by pulsed excimer laser photolysis of gaseous diatomic molecules. These medium hot atoms cause vibrational excitation of stable molecules during collisions, or react chemically to form products inaccessible to thermally cold species. Infrared fluorescence is being used to probe the broad spectral distribution of vibrationally and rotationally hot CO, CO_2, and CH_3F molecules produced in these atom-molecule encounters. An infrared laser diode is also employed to monitor, with a resolution of milliwavenumbers, the precise vibrational and rotational states excited during such collisions. Laser induced visible and U.V. fluorescence methods are being used to identify the species, and to measure the distribution of final states formed as a result of chemical reaction.

Dartmouth College
Hanover, New Hampshire 03755

181. Photoexcited Charge Pair Escape and Recombination
C.L. Braun, Dept. of Chemistry **$81,500**
(24 mo.)

The escape and recombination of charge pairs produced by photoexcitation of organic molecules is being studied. The recombination of geminate charge pairs formed by the photoionization of solute molecules in low dielectric constant solvents is found to occur in picoseconds. This process is being studied by pump-probe conductivity techniques. Picosecond absorption measurements of the recombination kinetics are planned. The data are being compared with a detailed theory of the diffusive recombination of geminate charge pairs. The second key goal is to understand the mechanism of charge pair escape in electronically excited electron-donor-acceptor materials. A number of donor-acceptor geometries are being explored in these solid state studies. The possible role of the lowest-energy, charge transfer state in the formation of separated charge pairs (current carriers) is of special interest. Steady-state and nanosecond pulse measurements of both photocurrents and fluorescence are being used to test mechanistic ideas.

Louisiana State University
Baton Rouge, Louisiana 70803-0301

182. Theoretical Studies of Electron and Proton Transfer Processes in Fluids
N.R. Kestner, Dept. of Chemistry **$60,000**

This research program is designed to study electron and proton transfer processes in fluids, especially those which could be important in energy conversion. General theoretical studies are probing the role of temperature, pressure, and solvent effects on electron transfer rates. Our special attention is directed to such effects for reactions in the abnormal, or highly exothermic regions. Related work is exploring structure-activity relations, which are important in the related proton transfer processes. The general theories are being applied to specific reactions. In this regard, we are determining very accurate water-water interactions and other intermolecular potentials, exploring in detail the role of basis set errors. These are being used to obtain accurate interaction energies between electron transfer species such as Fe(II) and Fe(III) in aqueous solutions. Other studies are directed at predicting electron transfer rates in glasses, and highly viscous media.

Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

183. Photochemical Energy Storage: Studies of Inorganic Photoassistance Agents
M.S. Wrighton, Dept. of Chemistry **$270,000**

Light-driven, energy-storing chemical reactions are the object of study in this research program. Emphasis is on the use of semiconductor electrodes as the photoassistance agents for redox reactions such as the oxidation and reduction of H_2O. Fundamental studies of the nature of semiconductor/electrolyte interfaces to establish the energetics and kinetics for light-driven redox processes are one aspect of the program. Semiconductor materials under study in this connection include WS_2, InP, GaAs, Si, CdX (X = S, Se, Te), and amorphous hydrogenated Si. Another aspect of the program is chemical derivatization of the semiconductor surface for the purpose of improving durability and kinetics for the desired redox reaction. In the area of electrocatalysis, surface modification with metals, oxides, and polymers is being studied. Catalysis of halide oxidation and H_2O reduction have received most attention. Exploratory studies to find unique interactions of redox reagents with semiconductor electrode surfaces, such as I_3^-/I^- with n-WS_2, are in progress. Such unique interactions are likely to lead to high efficiency for energy conversion and specific redox processes.

Mount Holyoke College
South Hadley, Massachusetts 01075

184. The Study of the Photochemistry of Organic Dyes at Semiconductor Electrodes Using Total Internal Reflection Techniques
M.T. Spitler, Dept. of Chemistry **$65,399**

The photochemistry of organic dyes adsorbed at semiconductor surfaces is being studied through a combination of photoelectrochemical and total internal reflection techniques. The utilization of an attenuated total reflection method enables an *in situ* determination of the quantum efficiency of current producing photoreactions. The photochemistry of dyes at ZnO, TiO_2, and $SrTiO_3$ single crystal surfaces is being investigated using dyes that show significant triplet character or tendency to form aggregates. Selected photoreactions will also be studied at surfaces chemically modified in differing regions of donor and acceptor to serve as a model for catalytic photoreactions at powders.

National Bureau of Standards
Washington, District of Columbia 20234

185. Support of Critical Data Compilations

D.R. Lide, Jr., Office of Standard Reference Data **$200,000**

The Office of Standard Reference Data of the National Bureau of Standards administers a collaborative interagency program for the preparation of compilations of physical and chemical reference data. Current projects within the scope of the Division of Chemical Sciences fall in the following areas: physical and thermodynamic properties of fluids, solubility, electrolyte properties, gas-phase chemical kinetics, hydrocarbon properties, atomic data relevant to fusion, and thermodynamics of high-temperature systems. The approach is to review critically all relevant data from the literature, compare with theory, and select the most reliable values. Whenever possible, correlations are developed which allow prediction of unmeasured properties. Reviews are in press on high-temperature vaporization of alkali metal oxides, water solubility of polynuclear aromatic compounds, electrochemical equilibria in carbon-oxygen systems, and other topics.

186. Pulse Radiolytic Studies of Inter- and Intramolecular Electron Transfer Processes

P. Neta, Center for Chemical Physics **$135,000**

Studies of both intermolecular and intramolecular electron transfer processes are conducted using pulsed electron sources to generate the reactive intermediates, and time resolved absorption spectrophotometry to follow the kinetics of the ensuing reactions. Quantitative results are obtained, detailing the effects on the rates of intramolecular electron transfer of the charge distribution within the molecule, electron affinities of substituents, steric effects, and other structural parameters. Intramolecular electron transfer reactions within metalloporphyrins are also studied, because of the importance of these molecules in photosynthesis, and because they allow a detailed analysis of the effect of driving force and other parameters on the rates of these processes. The mechanism and thermodynamics of intermolecular electron transfer reactions are studied, using measurements of rate and equilibrium constants as a function of temperature to obtain quantitative information about activation energies, enthalpy, and entropy changes associated with these processes. Comparison of values of liquid and gas phase systems will permit a more quantitative understanding of solvation effects in electron transfer processes. Electron transfer reactions of metalloporphyrins and their anion- and cation- radicals with a variety of other chemical systems and especially with certain metal catalysts are being studied as models for understanding artificial photosynthesis and other photchemical processes involving porphyrins.

Ohio State University
Columbus, Ohio 43210

187. Pulse Radiolysis Studies of Fast Reactions in Molecular Systems

L.M. Dorfman, Dept. of Chemistry **$22,000**

The broad objective of this research project is to come to an understanding of the rates and mechanisms of chemical reactions induced by ionizing radiation. At the same time, the information generated about the reactive intermediates (free radicals, molecular cations, and anions) is of interest in other areas of chemistry as well. Reaction is initiated by a high energy electron pulse of submicrosecond duration, and the reactive intermediates are directly observed by fast optical absorption measurement (time resolution 5 nanoseconds). These observations also provide the optical spectra of the reactive transients. Systems presently under study are organic molecular cations and anions in solution, where the ions, important in radiation-induced reactions, also play a key role in cationic polymerization. Since the reactions are initiated by high energy electrons, the results obtained relate directly to radiation chemistry.

188. Kinetics of Fast Reactions of Excited Species

R.F. Firestone, Dept. of Chemistry **$82,000**
(14 mo.)

The project objective is identification of mechanisms for growth and decay of excited rare gas atoms and excimers in the presence and absence of foreign quenching agents, using pulse radiolysis methods. Identities of excited atomic precursors of bound excimer states are sought by modeling of a multi-stage reversible collisional relaxation mechanism for rovibrationally excited excimer molecules, in conformity with temporal behavior of excited atoms and rovibrationally relaxed excimers. Monitoring of excited species is done by emission spectrometry and tunable cw laser spectrophotometry. Kinetic parameters of selected 1s-2p state pairs are to be obtained by cw pumping, coupled with absorption measurements at low power densities, and at power densities sufficiently great to induce bleaching of the transition.

Oregon Graduate Center
Beaverton, Oregon 97006

189. Fundamental Studies in Charge Separation At Interfaces in Relation to Water Photolysis

J.K. Hurst, Dept. of Chemical, Biological & Environmental Sciences **$90,000**
(16 mo.)

This research is directed toward improving our conceptual understanding of the influence of microphase separation and compartmentation upon photostimulated redox processes. Three distinct activities are encompassed by these studies: (1) examination of mechanisms of transmembrane redox bilayer membranes; (2) development of inorganic two-photon excitation schemes for transmembrane charge separation; and (3) development of reversed micellar assemblies for water photolysis. Redox systems under study which exhibit net electron exchange across bilayers include lecithin-bound amphiphilic 4-alkylpyridinepentaammineruthenium$^{2+/3+}$ ions and dihexadecylphosphate-bound alkylviologen$^{+/2+}$ ions. Studies in two-photon excitation are based upon photoreduction of cupric ion to cuprous π-complexes which are capable of long-range photoinitiated electron transfer to oxidant sites. In reversed micelles, the relationship between O_2 and H_2 yields, and the topographic organization of Zn(II) porphyrin sensitizers, viologen charge relays, and colloidal RuO_2 and Pt sols is being explored. For all photoinitiated systems, pulsed laser spectrophotometry is being used to probe reaction dynamics.

Pennsylvania State University
University Park, Pennsylvania 16802

190. The Free-Radical and Ion Chemistry of Volatile Silanes, Germanes, and Phosphines

F.W. Lampe, Dept. of Chemistry **$104,000**

This research project consists of experimental studies of the chemical reactions initiated by the irradiation of gaseous silanes and germanes with electrons, infrared laser radiation, and vacuum-ultraviolet light. From the experimental studies fundamental reaction mechanisms relative to this new and unexplored chemistry are developed. In particular, the knowledge and understanding developed enables us to attempt useful exploitations of photochemical and radiation chemical techniques for the synthesis of amorphous solids of silicon, germanium, and mixtures thereof. Presently under study is the infrared laser photochemistry of SiH_4-HCl and SiH_4-GeH_4 mixtures, CH_3SiH_3, the vacuum-ultraviolet photochemistry of GeH_4 and SiH_4-GeH_4-NO mixtures, as well as the ion chemistry of SiH_4-CH_3Cl, SiH_4-CH_2Cl_2, SiH_4-$CHCl_3$, SiH_4-CCl_4, and CH_4-HCN mixtures.

Princeton University
Princeton, New Jersey 08544

191. Photoelectrochemistry With Chemically Modified Electrodes

T.G. Spiro, Dept. of Chemistry **$85,000**

The electrochemistry and photoelectrochemistry of metalloporphyrin electrode films is being explored, with a view toward catalyzing useful energy storage reactions, including the splitting of water to H_2O_2. Stable metalloprotoporphyrin films have been prepared via electroinitiated polymerization of the vinyl sidechains, and other porphyrin polymerization schemes are being explored. Cobalt porphyrins are being applied to the catalysis of H_2 production from water. The kinetics of the catalysis have been investigated in homogeneous solution using electrochemical techniques, and cobalt porphyrin electrode films have been developed, which are capable of sustained H_2 production, and their characteristics are being explored. Iron, chromium, and manganese porphyrins are being explored in oxidative chemistry, with the eventual aim of catalyzing water oxidation.

Purdue University
West Lafayette, Indiana 47907

192. Study of the Motion of Electrons in Non Polar Classical Liquids

G. Ascarelli, Dept. of Physics **$69,000**

In our study of the properties of electrons injected into a liquid, we have calculated the expected drift mobility in liquid Ar assuming that the primary scattering mechanism is due to thermal phonons. In this case, the deformation potential that appears in the expression for acoustic phonon scattering is $\Xi = -n(dV_0/dn)$. To take into account the fact that we are considering an electron moving in a liquid, rather than a crystal, we considered the density fluctuations in a volume whose dimensions are equal to the thermal wavelength of the electron. These fluctuations assure that the mobility remains finite even when $dV_0/dn = 0$. Their effect is also to increase the mobility near the critical point by decreasing the phonon amplitude inside of a density fluctuation where the electron is located. The resulting mobility near the critical point, assuming $m^* = m_0$ is $1900 cm^2/Vs$ decreasing to $500 cm^2/Vs$ when the density is $1.5x10^{22} cm^{-3}$. A maximum mobility of $5000 cm^2/Vs$ is predicted where $dV_0/dn = 0$ and a mobility equal to $50 cm^2/Vs$ is predicted at the critical point. Our preliminary Hall mobility measurement in Ar at a density $2x10^{22} cm^{-3}$ is $1600 cm^2/Vs$. From it, a drift mobility of $1355 cm^2/Vs$ is calculated. This value is in excellent agreement with the phonon scattering calculation ($1340 cm^2/Vs$) alluded to above.

Stanford University
Stanford, California 94305

193. Energy Transfer Processes in Solar Energy Conversion

M.D. Fayer, Dept. of Chemistry **$110,000**

This project is examining energy transport processes in nontraditional systems, using picosecond and other optical techniques and statistical mechanical theoretical methods. There are a wide variety of situations in both natural and man-made systems which cannot be modeled as periodic arrays of molecules. In many systems, inherent disorder and characteristic size and shape play key roles in determining energy dynamics. We have developed the first accurate and detailed statistical mechanics theory of energy transport in disordered systems with finite volume. We are using a picosecond transient holographic grating technique, and picosecond fluorescence mixing methods with conventional fluorescence and absorption experiments to study energy transport among dye molecules attached to long hydrocarbon chains organized in micelle solution, and to examine energy transport in chromophore containing polymers. These clustered chromophore systems permit extremely high local chromophore concentrations (and therefore efficient energy transport), without the normal energy quenching associated with conventional concentrated dye solutions. In addition, we are studying electron transport in disordered systems. Using piosecond lasers, electron transport between organic molecules is examined on a timescale fast enough to show the dynamical details important in natural and laboratory chemical electron transfer reactions. Electron transport in amorphous silicon is under investigation with transient grating techniques.

194. Fundamental Electron Transfer Processes At the Semiconductor/Liquid Interface

N.S. Lewis, Dept. of Chemistry **$150,000**
(24 mo.)

Variations in fundamental electron transfer parameters at the semiconductor/liquid interface are studied with systematic changes in bulk semiconductor composition in the $GaAs_{1-x}P_x$ and $Al_{1-x}Ga_xAs$ series of alloys. We have obtained single crystal, epitaxially grown, n-type samples of representative members of these series, and have investigated changes in electrode properties in both aqueous and nonaqueous solvents. In aqueous selenide-containing solutions, we observe stable photoanode behavior for all members of the series, and observe high spectral response characteristics for all materials. Similar behavior is found in nonaqueous solvents, and in both solvent systems the photoanode properties seem more strongly correlated to the bulk semiconductor band gap than to the actual bulk or surface composition of the electrode. More detailed measurements on the variation of properties in this system are in progress.

Temple University
Philadelphia, Pennsylvania 19122

195. Dynamic Aspects of the Dye-Sensitized Photoconductivity of Semiconductors
A.M.P. Goncalves, Dept. of Chemistry **$80,000 (14 mo.)**

The objective of this program is to probe the dynamics of the elementary processes (injection, recombination, and escape) which determine the efficiency of dye-sensitized semiconductor/electrolyte solar cells. The general experimental approach relies primarily on the use of subnanosecond time-resolved spectroscopic techniques: fluorescence and transient absorption or gain. The fluorescence lifetimes of several dyes adsorbed on semiconductors and insulators at high surface coverage (measured with streak camera detection) are on the order of 50 picoseconds, as much as 30 times shorter than in solution. The fact that a similar lifetime reduction occurs for each dye, both on semiconductor and insulator surfaces, suggests that energy transfer quenching is primarily responsible for the short lifetimes. This is confirmed by fluorescence quantum yield measurements as a function of surface coverage: in the limit of very low surface coverage, the quantum yield approaches the solution value on an insulator and a much smaller value on a semiconductor. These experiments indicate that injection occurs in a time on the order of 150 ps. More recent measurement of the flourescence lifetimes at very low surface coverage (using a time-correlated single photon counting technique) have provided a much more reliable direct measurement of the injection time: 400 ps.

University of Alabama
Tuscaloosa, Alabama 35486

196. ELDOR Investigations of Radiation Processes
L.D. Kispert, Dept. of Chemistry **$66,700**

The objective of this research is determine how a lattice affects energy transfer and primary radiation and photochemical processes in irradiated organic crystals and glasses. Such information is vital to understanding photosynthesis, photoinduced solid-state polymerization, electron and hole transport, and stereospecific reactions in solids. Electron spin resonance, electron-nuclear double resonance, and electron-electron double resonance techniques are being used to identify the molecular fragments formed and to detect the energy transfer processes that occur. In particular, selected sugar, polyalcohol, carboxylic acid, and acetamide crystals are being studied to determine the effect of hydrogen bonding on radical stability and reaction mechanisms as a function of temperature in crystals containing (1) varying crystallographic forms, (2) rotational disorder, and (3) impurities. Preexisting electron traps, first observed by this research, have been studied in crystals of rhamnose and trehalose, radical intermediates have been identified in irradiated beta-carotene, photoexcited triplet state lifetimes have been measured, and halogenated organic anions have been detected.

University of Arizona
Tucson, Arizona 85721

197. Mechanisms of Photochemical Energy Conversion By Chlorophyll
G. Tollin, Dept. of Biochemistry **$160,600 (24 mo.)**

The goals of this project are to elucidate the detailed mechanisms involved in light-induced one-electron transfer reactions involving chlorophyll (and related compounds) and electron donors and acceptors, and to determine the interactions between the elementary steps in these processes and environmental parameters such as viscosity, dielectric constant and homogeneous vs. heterogeneous reaction matrices. The intent is to develop a body of fundamental information which can be used to devise strategies for increasing the yields of the high energy products of such reactions, to physically separate these products and to decrease the probability of recombination (i.e., back reaction), and to facilitate secondary electron transfer to external donors and acceptors. Current work involves the use of laser flash photolysis to monitor excited state and radical dynamics in lipid bilayer vesicle systems.

University of California/Irvine
Irvine, California 92717

198. Research in Chemical Kinetics
F.S. Rowland, Dept. of Chemistry **$180,000**

This research project is directed toward the understanding of the rates and mechanisms of chemical reactions, including some of interest to atmospheric chemistry. The reactions of thermalized ^{18}F and ^{38}Cl atoms with gaseous $(CH_2{=}CHCH_2)M$ compounds are being studied for M = Sn, Ge, Si, C to determine the extent of restricted intramolecular energy flow ("non-RRKM") in such systems. Reactions of halogen atoms with haloolefins (X + $CH_2{=}CHY$; X = F,Cl; Y = F,Cl,Br) are furnishing rate information about radical lifetimes, and mechanistic information such as selectivity and isomerization. The temperature dependence of ^{38}Cl reactions with olefins is being studied over the 240-360 K temperature range. The mechanism of the direct gas-phase photolysis of $^{14}CS_2$ is being investigated with and without O_2 present. The rates and mechanisms of hydrolysis in aqueous solution are being measured for gases occuring in the atmosphere, including OCS, CH_3I and CH_3Br. The gas phase photolyses of PH_3 and P_2H_4 and the co-photolysis of PH_3 and NH_3 are being investigated. The possibility of hot Cl abstraction by energetic ^{38}Cl atoms is being tested.

University of California/Los Angeles
Los Angeles, California 90024

199. Time-Resolved Laser Studies On the Energy Transfer and the Configurational Changes in Bacteriorhodopsin
M.A. El-Sayed, Dept. of Chemistry **$100,000**

Bacteriorhodopsin (BR) is another photosynthetic system besides chlorophyll. While chlorophyll uses electron pump, BR uses proton pump. The understanding of storing solar energy via proton pumps is of vital importance. Thus the understanding of the primary photochemical and photophysical process in BR is of vital current interest. We developed time-resolved resonance Raman and optical techniques in order to record the spectra of the different transients formed following the initial photosynthetic absorption process. Questions such as: (1) does energy migration take place to specific sites prior to photochemistry; (2) does isomerization of retinal take place on the picosecond time scale; and (3) how does the Schiff base lose its proton during the photochemical cycle, are among the questions we are attempting to answer. Very recently, we started using time-resolved optical spectroscopy of the protein and the retinal systems, to identify the nature of the coupling between these two systems which is undoubtedly responsible for the proton pumping required for photosynthesis in bacteriorhodopsin.

University of California/Santa Barbara

Santa Barbara, California 93106

200. *Energy Transformations in Transition Metal Complexes*

R.J. Watts, Dept. of Chemistry **$89,300**

The projects in this program are intended to explore basic photochemical and photophysical phenomena in transition metal complexes. Five primary areas of endeavor include: (1) photochemical and photophysical consequences of metal-carbon bonding to acceptor ligands with extended π-systems; (2) electronic relaxation phenomena between excited states of metal complexes; (3) mechanisms of excited state electron transfer reactions; (4) tuning of electronic excited states by extension of π-conjugation in N-heterocyclic ligand-metal complexes; and (5) photochemistry and photophysics of organometallic sandwich complexes. Techniques being applied in these projects include time-resolved emission spectroscopy, laser-induced transient and excited state absorption spectroscopy, and ^1H and ^{13}C nmr spectroscopy. Laser double resonance techniques are presently being developed for the purpose of characterizing electronic relaxation between excited states of metal complexes. Synthesis and characterizations of complexes containing metal-carbon bonds are being carried out in order to facilitate the projects in area (1) above. The emission spectroscopy and photoinduced electron transfer reactions of several of these complexes are presently under investigation.

University of Colorado

Boulder, Colorado 80309

201. *Chemical Probes of Charge Transfer At Semiconductor/Liquid Junctions*

C.A. Koval, Dept. of Chemistry **$75,000**

The surface energetics for p- and n-InP/CH_3CN and p- and n-WSe_2/CH_3CN interfaces are being carefully examined with capacitance measurements. This information is used to interpret the kinetic aspects of voltammograms obtained at these electrodes for a series of metallocene$^{+,0}$ redox couples. Complexes with the general formula $Cr(III)(NH_3)_5(RCO_2)^{2+}$ are being examined for use in experiments to detect non-thermalized, photogenerated electrons (hot carriers). Metallocenes with charged substituents ($-NR_3^+$, $-COO^-$) are used to investigate diffuse-layer effects at semiconductor/liquid junctions. These experiments are designed to delineate fundamental kinetic aspects of charge transfer at semiconductor/solution interfaces, with the ultimate goal of improving efficiencies and lowering costs for devices based on photoelectrochemical cells.

University of Florida

Gainesville, Florida 32611

202. *Radiation Chemistry of Hydrocarbon and Alkyl Halide Systems*

R.J. Hanrahan, Dept. of Chemistry **$71,000**

Current work is directed towards understanding the mechanism of product formation in the gamma and pulsed electron radiolysis of simple chemical systems. Studies of the radiolysis of hydrogen-carbon monoxide mixtures on alumina surfaces include measurement of both hydrocarbon and oxygen-containing products; certain yields are increased by 100 times or more in comparison to the gas phase. The radiolytic oxidation of propane shows many similarities to auto-oxidation in products and reaction pathways; computer modeling of the reaction scheme accounts for the oxygen pressure dependence of product yields. Measurements are being made on the rates of attack of OH radicals on hydrocarbon and halocarbon gases, using the pulse radiolysis method. Comparison of results at high and low water concentration yields data on the rates of OH + radical combination reactions in these systems. Photolysis of methyl iodide-perfluoromethyl iodide mixtures forms several products, including: (1) methane and perfluoromethane; (2) ethane and perfluoroethane; and (3) several mixed products such as trifluoromethane, difluoroethylene, and trifluoroethane, along with HI and HF.

University of Houston

Houston, Texas 77004

203. *Charge Separation in Photoredox Reactions*

L. Kevan, Dept. of Chemistry **$90,000**

The objective of this research is to probe the molecular mechanistic and structural aspects of charge separation in photoredox reactions in micellar and vesicle systems in order to eventually couple this charge separation to chemical energy storage. Tetramethylbenzidine (TMB) has been photoionized to produce the cation radical in liquid and frozen micellar solutions of anionic, cationic, and nonionic surfactants, and in liquid and frozen synthetic, anionic, and cationic vesicle solutions. The cation is observed by optical absorption, electron spin resonance, and electron spin echo spectrometry. Cation-water interactions, detected by electron spin echo modulation analysis, indicate that the photoproduced cation is located asymmetrically within both the micellar and vesicular structures, and generally correlates with photoionization efficiency. Micelle surface modification by added salts and varying counterions has led to some control of photoionization efficiency. The decay kinetics of photoproduced cations in micelles have been found to be characterized by time dependent rate constants.

University of Massachusetts

Boston, Massachusetts 02125

204. *Investigation of the Structure of Photosynthetic Reaction Centers*

H. van Willigen, Dept. of Chemistry **$68,500**

The structure of photosynthetic reaction centers and model systems is studied with the aid of magnetic resonance techniques and optical spectroscopy. Research has focused on the application of Electron Spin Resonance (ESR) in the study of photo-excited triplets of a series of porphyrins. The spectroscopic data give information on the structure of aggregates of these systems and give an insight into their photophysical and photochemical properties. The study is concerned as well with the application of Electron Nuclear Double Resonance (ENDOR) in the study of the electron spin distribution in the photo-excited triplets. The method has been used to measure hyperfine interactions in the photo-excited triplets of the primary donor in reaction center preparations of photosynthetic bacteria.

University of Minnesota
Minneapolis, Minnesota 55455

205. *The Contribution of Electronically Excited States to the Radiation Chemistry of Organic Systems*

S. Lipsky, Dept. of Chemistry **$100,000**

A general study is being made of those photophysical properties of organic molecules that have relevance in determining their radiation-chemical behavior. Projects currently in progress include: (1) a study of the dependence on scavenger concentration of the efficiency of quenching geminate-ion recombination fluorescence of saturated hydrocarbon liquids, in order to characterize the distribution of electron-positive ion separation distances; (2) a study of the dependence on photon energy of the probability of photoionization and of the average range of the electron ejected from aromatic solutes in non-polar fluids, via comparison with theory of the effect of an electric field to reduce the geminate-ion recombination fluorescence; (3) a study of the effect of perfluorocarbons to alter the distribution function of electron-positive ion separation distances by interaction with epithermal electrons as manifested by an altered electric field dependence of photocurrent.

University of Nebraska
Lincoln, Nebraska 68588-0304

206. *Electrochemical and Optical Studies of Model Photosynthetic Systems*

T.M. Cotton, Dept. of Chemistry **$75,000**

A combination of electrochemical and resonance Raman techniques, supplemented by ultraviolet-visible spectroscopy, is being used to characterize some important properties of the pigments of the bacterial photosynthetic reaction center. Characterization includes determination of the redox states of the various components during the initial photoact as well as the identity and spectral character of the neutral and charged species involved. Much of the present knowledge of the primary photoact in photosynthesis is based on *in vitro* measurements or on *in vivo* measurements which are subject to ambiguous interpretation. The present approach uses innovative techniques in an attempt to overcome some of the drawbacks of previous studies. Attempts are under way to incorporate bacteriochlorophyll, bacteriopheophytin, and quinones from reaction centers into monolayer arrays. In these designed monolayer constructions the orientation, spacing, and identity of the included components are under a high degree of control. Electrochemical and spectral studies of the monolayer systems should provide new insights regarding the effect of structure on the optical and redox properties of these molecules.

207. *Energetics of the Formation and Reactions of Gaseous Ions*

G.G. Meisels, Dept. of Chemistry **$85,000**

Two areas are addressed in this research program. One area uses threshold photoelectron - coincident photoion mass spectrometry to study ions whose internal energies are known within 0.025 eV. The other area derives the spatial distribution of ionization by 100 to 1000 eV electrons from ion residence times in the chemical ionization source of a mass spectrometer. In the first area, the energetics of the formation, isomerization, and fragmentation of gaseous cations are measured. Anisole and dimethylether show stable molecular ions several eV above fragmentation onset, and thus do not, at all energies, behave in accordance with statistical theories. In the second area, linear ionization rates are measured as a function of beam penetration into the ion source; they increase briefly from the point of beam entry and then decrease smoothly. Ranges derived from them for methane, nitrogen, and the rare gases lie between those measured by bulk techniques and the probable electron path length. The coaxial geometry and preferential detection of ions formed along the beam axis permit evaluation of both longitudinal and radial distributions of ion formation.

208. *High Energy Halogen Reactions Activated By Nuclear Transformations*

E.P. Rack, Dept. of Chemistry **$71,600**

The functional goal of this project is to understand better the chemical reactivity of high energy monovalent species. High energy reactions of halogen atoms or ions activated by nuclear transformations are studied in gaseous, high pressure, and condensed phase saturated and unsaturated hydrocarbons, halomethanes, and liquid and solid aqueous solutions of biological molecules. Specifically, the stereochemistry involving single chiral center molecules, systematics, mechanisms, and halogen reactivity in a collapsing molecular environment, and caging of hot atoms in an ice lattice are under investigation. The stereochemistry of exothermic halogen atom homolytic bimolecular substitution ($^{S}H^{2}$) at the chiral centers of chiral 2-halopropionyl halides is currently studied. Practical applications of recoil atom chemistry to activation analysis or molecules in biological or environmental systems, to radiopharmacy involving synthesis and radioprotection, and to the study of solute-solute and solute-solvent interactions of dilute aqueous solutions of biological molecules are being carried out.

University of North Carolina
Chapel Hill, North Carolina 27514

209. *Energy Conversion Processes Based On Molecular Excited States*

T.J. Meyer, Dept. of Chemistry **$105,000**

This research effort is based on the study and exploitation of excited states of transition metal complexes. A particularly important goal is the design and characterization of new classes of photosensitizers, and their application to solar energy related problems. In technical detail the work involves the measurement of the photochemical and photophysical properties of excited states, the application of theory to such processes, synthesis of new types of potential photosensitizers, the preparations and properties of metallopolymers containing metal complex chromophores, the study of electron and energy transfer processes of the photosensitizers in solutions and polymeric films, and possible applications of these materials in photochemical and photoelectrochemical energy conversion processes.

University of North Carolina at Charlotte
Charlotte, North Carolina 28223

210. *Oligomer and Mixed-Metal Compounds, Potential Multielectron Transfer Catalysts*

D.P. Rillema, Dept. of Chemistry **$60,100**

The goal of the project is to design and characterize new classes of photosensitizers and their application to solar energy conversion. Current work involves characterizations of fundamental precursors that will be used (1) to prepare molecules that contain a coordinatively unsaturated metal complex connected to a photoactive electron transfer metal chromophore, and (2) to synthesize multi-metal complexes capable of "simultaneous" multielectron transfer. The characterizations include: (1) isomer separation of metal complexes containing assymetric ligands; (2) thermodynamic studies of ground state and excited state redox properties; (3) assessment of the relative energy positions of heterocyclic ligand π^* energy levels and their exploitation for the preparation of new light-sensitive chromophores; and (4) photophysical investigations of the excited state energies, lifetimes, and electron transfer properties of the photochromophores.

University of Puerto Rico
Mayaguez, Puerto Rico 00708

211. *Photoelectrochemistry of New Phenothiazine Dye Derivatives*

F.A. Souto, Dept. of Chemistry **$125,000 (24 mo.)**

This project has been designed to explore the potential of amphiphilic derivatives of thionine for the study of photochemical and other energy conversion systems in aqueous solution. Emphasis is placed on the synthesis and identification of lipophilic, amphiphilic, and hydrophilic derivatives of thionine. These dyes have a great potential to alleviate the problems that prevent efficient electron-transfer quenching from taking place in concentrated solutions of photoredox couples. Our approach to this fundamental aspect of photoelectrochemistry consists in the study of the photophysical, photochemical, and electrochemical processes involved in the electron-transfer quenching of excited amphiphilic organic dyes solubilized within surfactant micellar assemblies. The initial results on the aggregation of thionine and its disulfonated derivatives indicate that their kinetic properties and thermodynamic characteristics are highly dependent on their ionic character and distribution of polar groups on the periphery of the phenothiazine nucleus. Therefore, a considerable experimental effort has been devoted to the unambigous identification of each derivative. High frequency (470 MHz) ^{1}H NMR spectra for each derivative in monomeric form has been the key to the solution of this activity. The photochemical and electrochemical characterization of these derivatives is in progress at this time. The indication is that 4,6-disulfonated thionine is the preferred isomer for its kinetic characteristics.

University of Rochester
Rochester, New York 14627

212. *Applications of Photo-Induced Electron Transfer and Hydrogen Abstraction Processes to Chemical and Electrochemical Conversion Processes*

D.G. Whitten, Dept. of Chemistry **$190,000 (24 mo.)**

This research program involves studies of photochemical redox reactions occuring via electron transfer and hydrogen atom abstraction processes initiated by excitation of chromophores absorbing visible and near ultraviolet light. A part of the project involves direct study of photochemical reactions and external factors that can modify them. In addition, photoelectrochemical processes based on them are being investigated. Our studies of direct photochemical reactions have recently focused on photoredox reactions of certain indigo dyes. These dyes undergo net photoreduction processes with a variety of electron donors by, in some cases, a multiplicity of mechanisms. Among the most interesting mechanisms is a net hydride ion transfer that occurs via a sequence of electron, proton, and second electron transfer, all within the initially formed encounter complex. We are also investigating the effect of inclusion complex formation on reactivity using various amylose derivatives as selective hosts for a variety of reactive substrates. The photoelectrochemical studies are currently focusing on hydrogen atom abstraction reactions from alcohols occuring with substrates excited by visible light.

University of Tennessee
Knoxville, Tennessee 37996-1600

213. *Studies of Radiation-Produced Radicals and Radical Ions*

T.F. Williams, Dept. of Chemistry **$96,000**

The basic objective of this project is to characterize important free radical and radical ion intermediates generated by irradiation of molecular systems. Current emphasis is being placed on the radical ions produced in the primary chemical processes resulting from the absorption of high energy radiation. Novel radical ions derived from typical saturated molecules are being generated and stabilized in suitable solid matrices, examples being fluorocarbon radical anions in hydrocarbon matrices and the radical cations of alkanes, ethers, and organometals of Group IVB alkyls in fluorocarbon matrices. Electron spin resonance (ESR) spectroscopy is used to identify these paramagnetic species. Measurements of hyperfine coupling constants, including those of ^{13}C-labeled radicals, provide information about geometrical structure and spin density distribution. The chemical rearrangement of positive ions is also being investigated. Studies are also underway on the generation and characterization of organometallic radicals and radical ions in systems which are relevant to catalysis and solar energy conversion.

University of Texas
Austin, Texas 78712

214. *Organic Redox Phototransformations at Chemically Modified Surfaces*

M.A. Fox, Dept. of Chemistry **$70,000**

Exploratory and mechanistic studies of new chemical transformations of organic molecules at native and chemically modified surfaces represent the goal of this research program. New electrode materials are being prepared by adsorption, covalent attachment, polymerization, and mulling with electroactive or light-sensitive materials; and physical studies of the properties of these materials are being conducted. Both photocatalytic and photosynthetic organic reactions can be initiated by electron exchange induced by visible light excitation of either native or chemically modified semiconductor surfaces. Several spectroscopic techniques are being used to evaluate intermediates and surface states: (1) Fourier transform infrared spectroscopy; (2) Resonance Raman spectroscopy; (3) laser-induced flash coulostatic measurements; (4) photochemically induced magnetic resonance; (5) picosecond laser spectroscopy; (6) rotating ring disc electrochemical techniques; and (7) ESCA and Auger spectroscopy. New metal non-oxides and p-type semiconductors are also being investigated, and the search for new reactions on these novel materials is continuing.

Washington University
St. Louis, Missouri 63130

*215. **Reaction Studies of Hot Silicon and Germanium Radicals***
P.P. Gaspar, Dept. of Chemistry **$93,000**

The goal of this research project is to discover: (1) what are the reactions of high energy Si and Ge atoms; (2) how do the reactions take place; and (3) how are the reaction pathways influenced by the energy and electronic state of the free atoms, and of the reactive intermediates that they produce. Silicon and germanium atoms are formed at high energies by nuclear transformations such as $^{31}P_{(n,p)}{}^{31}Si$ and $^{76}Ge_{(n,2n)}{}^{75}Ge$, and at low energies by thermal evaporation. Intermediates such as SiH_2 and $GeMe_2$ are generated by pyrolysis and photolysis. In the past year the silylsilylene-to-disilene rearrangement has been demonstrated in a hot-atom experiment. Unsubstituted H_3Si-^{31}Si-H from reaction of recoiling silicon atoms with silane has been shown to rearrange to $H_2Si{=}^{31}SiH_2$, which was trapped with butadiene. The mechanism of addition of silylenes to 1,3-dienes has been established as consisting of a concerted 1,2-addition followed by competing Si-C and C-C bond cleavages in the opening of the silirane ring. Rate measurements on the reactions of two silylenes, Me-Si-Ph and Me_2Si, have been carried out by laser flash photolysis.

Wayne State University
Detroit, Michigan 48202

*216. **Dynamics of Charge-Transfer Excited States Relevant to Photochemical Energy Conversion***
E.C. Lim, Dept. of Chemistry **$76,800**

The purpose of this research is to gain fundamental understanding of radiationless transitions in exciplexes and charge-transfer complexes, which are pertinent to photochemical energy conversion. Both the steady-state and time-resolved measurements of fluorescence and triplet formation are employed to study factors which influence various nonradiative decay channels in condensed phase. The results indicate that the dominant nonradiative decay channel of these species at moderately high temperatures (room temperature and above) may be internal conversion to the ground state. They also suggest that there is a propensity rule for singlet→triplet intersystem crossing in charge-transfer complexes. Thus, singlet→triplet intersystem crossing from a charge-transfer singlet state appears to be efficient only when a locally excited triplet state of a component molecule (donor or acceptor) lies below the charge-transfer singlet state, consistent with vanishingly small spin-orbit coupling between charge-transfer states.

Chemical Physics

Aerodyne Research, Inc.
Billerica, Massachusetts 01821

*217. **A Study of CH Reactions Relevant to Combustion/Gasification Processes***
J.A. Silver, G.W. Stewart, Center for Chemical and Environmental Physics **$88,200**

Little is known about the reactions of monovalent carbon radicals known as carbynes, and in particular, those of CH radicals. Yet they play an important role in the chemistry of combustion and gasification processes, including the formation of NO_x via the prompt-NO mechanism. They also appear to serve well as a testbed for studying the mechanistic behavior of four-center reactions, and appear to exhibit both abstraction and addition at different temperatures. We are involved in a project of basic research in which both rate constants and product distributions are determined from reactions of CH with other small molecules found in combustion streams. These studies are performed on a high temperature fast flow reactor, capable of operating between room temperature and 1500 K. The goal of this project is to improve our fundamental understanding of the chemistry of carbynes.

Brown University
Providence, Rhode Island 02912

*218. **Interactions of Molecules With Surfaces***
E.F. Greene, Dept. of Chemistry **$74,200**

The rate of desorption of Cs, K, Na, and Li atoms from the (100) and (111) surfaces of silicon is followed by surface ionization. The rates are markedly lower from surfaces stable in the temperature range 800-950K than they are from metastable ones supercooled below surface phase transitions. These are the well-known one for (111) at 1120±40K, and one for (100) at 980±20K. On the metastable surfaces the desorption is first order and the atoms appear to be highly mobile. On the stable surface where the desorption is mixed, first and second order the atoms are also highly mobile but concentrated at steps between terraces from which most of the desorption occurs. In a different experiment molecules of tetramethyldioxetane are given kinetic energy by being seeded into nozzle beams of hydrogen. This kinetic energy is converted by a single collision with a surface into internal energy of the molecules, which then can decompose and emit light. The amount of light varies with the kinetic energy, the temperature of nozzle, and the nature of the surface. This experiment offers an effective method of activating the decomposition of gaseous molecules.

California Institute of Technology
Pasadena, California 91125

219. *High Resolution Infrared Spectroscopy: Dynamics of Vibrationally Excited States*
K.C. Janda, Dept. of Chemistry **$68,000**

Molecular beam laser photodissociation spectroscopy is used to characterize intramolecular energy redistribution in excited vibrational states of molecules. Van der Waals molecules are used as prototypes for this effect because deposition of one infrared photon is enough to break a bond. The goal is to have a description of the internal molecular energy transfer in microscopic detail. It appears that vibrational predissociation of triatomic molecules is well described by Fermi's golden rule perturbation theory. This theory predicts that a HeI_2 molecule would have short-lived vibrationally excited states, 10^{-10} sec., while the $NeCl_2$ molecule would have long-lived vibrationally excited states, greater than 10^{-5} sec. This dramatic dependence of predissociation lifetime on molecular structure has now been observed. For larger molecules, simple theories do not seem to apply. For example, a series of constituents were bound to ethylene. The series included Ne, Ar, HF, HCl, NO, C_2H_4. In spite of the broad distribution of molecular structures and binding energies in this series, the vibrational predissociation lifetimes are all on the picosec. timescale. Recently, resolved rotational structure for the $Ne{\cdot}C_2H_4$ complex has been assigned as due to a hindered internal rotor.

220. *Studies in Spectroscopy and Chemical Dynamics*
A. Kuppermann, Chemistry & Chemical Engineering Division **$95,000**

Studies are being made on the low energy electron impact spectroscopy of molecules and free radicals of importance in combustion processes. The aim of these studies is to gain information about the low-lying electronically excited spin-forbidden states of these species and of their possible relevance to the reactions occuring in these processes. Studies are also being made on the dynamics of elementary reactions involving free radicals such as H or CH_3. Free radicals are produced by pulsed laser photolysis of a parent halide and an abstraction product of the reaction of the free radical with molecules such as C_2H_2 and HCN is detected by vacuum ultraviolet laser-induced fluorescence, using a second laser time-delayed with respect to the first one. The object of these studies is to obtain information about the translational energy dependence of the cross section of these reactions and its relation to activation energies. Such reactions are important in combustion processes.

Columbia University
New York, New York 10027

221. *Energy Partitioning in Elementary Gas Phase Reactions*
R. Bersohn, Dept. of Chemistry **$70,000**

The dynamics of the elementary reactions $A + BC \rightarrow AB + C$ and $A + BCD \rightarrow AB + CD$ are being studied by a two laser experiment. One laser generates the reactive atoms A (carbon, hydrogen, fluorine or sulfur) by photodissociation of a suitable parent molecule. The second laser probes the internal state distribution of the products. The reactions of fluorine atoms with HI, ICN and I_2 have been studied. All iodine atoms products are in the ground state. The conclusion is that fluorine atoms in their $J = 1/2$ state are unreactive. The hydrogen atom exchange reactions $H + DX \rightarrow HX + D$ are being studied ($X = Cl, F$). Spectroscopic techniques are being developed for studying the time dependence of atomic concentrations, in particular of different atomic sublevels.

Cornell University
Ithaca, New York 14853

222. *Shock Tube Pyrolysis of Automatic Hydrocarbons–Detection of Soot Precursors*
S.H. Bauer, Dept. of Chemistry **$51,000**

The objectives of the shock tube experiments are to determine the fragmentation patterns for structurally related di- and tricyclic aromatics, to measure the relative levels of soot produced, and to formulate semi-quantitative mechanisms for these processes. The experiments are performed in a single-pulse shocktube with a coaxial laser beam absorption diagnostic. Gas chromatographic analyses are made of samples extracted from the downstream end of the shock tube. During the test time attainable with this configuration (700-900 μs) conversion of the shocked samples is kinetically limited. The shapes of the He/Ne transmission curves indicate that the attenuation of the beam is not due to loss by scattering from the final product, but to absorption by precursor species, the concentrations of which first rise and then decline due to subsequent reactions. For recording their extended absorption spectra, the He/Ne laser was replaced by a black-body source, and the photodetector by a 3/4m spectrometer equipped with a multi-element array detector-amplifier-computer system. This configuration, now being tested, will allow simultaneous recording of absorption spectra at 20 adjacent spectral intervals (each 5nm wide) with a time resolution of 20μs, for the entire duration of the shock-quench period.

Georgia Institute of Technology
Atlanta, Georgia 30332

223. *Kinetic Study of Radical-Aromatic Hydrocarbon Reactions*
A.R. Ravishankara, Engineering Experimental Station **$64,700**

Improvements in the fundamental understanding of chemical reaction rates and pathways in radical-unsaturated and aromatic hydrocarbon reaction are the principal objectives of this program. Using the technique of (laser/flash) photolysis/(resonance/laser induced) fluorescence, the absolute rate constant measurements for reactions of H, O, OH + aromatic and olefinic hydrocarbon are being carried out as functions of temperature and pressure. By judicious interpretations of observed kinetic isotope effects, the yield and identity of certain products, the temporal profiles of reactant and product concentrations, and the effect of pressure and scavenger concentrations on the rate coefficients, the reaction mechanisms for all the above reactions in the temperature range of 250-1100 K are being elucidated. Futhermore, studies on aromatic free radicals using laser induced fluorescence have been initiated. Information gained from these studies is expected to improve utilization of hydrocarbons both as combustibles and as feedstocks for synthetic fuel production, as well as increasing our understanding of hydrocarbon combustion.

Howard University
Washington, District of Columbia 20059

224. *Laser Studies of the Dynamics of Atom Molecule Reactions*
W.M. Jackson, Dept. of Chemistry **$55,000**

This project uses tunable dye layers to measure the reaction rates of CN free radicals as a function of their internal energy. The project is based upon unique photochemical sources of internally excited CN radicals that can be produced from the laser photolysis of C_2N_2, ClCN and BrCN. Each of these compounds produce CN radicals that are rotationally or vibrationally hot. The amount of rotational and vibrational excitation depends upon the compound used, so that by measuring the rate constant with a particular source of CN, we hope to be able to obtain information about the effects of internal excitation on the rate constants for CN reaction. Studies have been completed on the effects of one quanta of vibrational energy on the rate constant for the reaction of CN with H_2, O_2, CO_2, N_2, HCN, C_2N_2, and CH_4. These studies are currently being extended to include the effects of larger amounts of vibrational energy in the CN radical. Other studies have been started which demonstrate that the quenching of a combination of translational and rotational energy can produce vibrational excited CN radicals with a high probability.

Illinois Institute of Technology
Chicago, Illinois 60616

225. *Theoretical Studies of Combustion Dynamics*
J.M. Bowman, Dept. of Chemistry **$64,700**

The objective of this research is to develop and apply approximate but accurate quantum mechanical methods to reactions of interest in gas phase combustion. Such a theory has been developed and applied to the reactions $O(^3P) + H_2$, $O + D_2$ and $O + HD$ using an acc*ab initio* potential energy surface. Extension of the theory to treat diatom + diatom reactions has been made, and the first application will be to the $OH + H_2$ reaction. A surface will be obtained from new *ab initio* calculations that are planned by Dr. Thom Dunning. Work is also underway to calculate the vibrational energies and lifetimes of HCO and HOCO using *ab initio* potential surfaces calculated by Harding. This work is based on a vibrational self-consistent field plus configuration interaction method developed here. The interaction of radiation with long-lived collision complexes is also being investigated, and preliminary calculations indicate that stabilization by stimulated emission may be feasible for small systems using lasers of moderate power.

226. *Studies of Combustion Kinetics and Mechanisms*
D. Gutman, Dept. of Chemistry **$150,000**

The purpose of the research is to gain new quantitative knowledge of the kinetics and mechanisms of the reactions of polyatomic free radicals which are important in hydrocarbon combustion processes. The free radicals are generated in a heated tubular reaction by the multiple-photon-induced decomposition of suitable precursors by a CO_2 TEA laser. The ensuing reactions are monitored using a photoionization mass spectrometer capable of recording the time evolution of either reactants or products. The recombination of C_2H_5 radicals is being studied in detail. Special procedures to determine their initial concentrations are also being developed. The reactions of alkyl radicals with molecules are being investigated as a function of pressure as well as temperature. In particular the $C_2H_5 + O_2$ reaction is being studied from 300-1000K and from 0.4 to 8 torr total pressure. Details of mechanism changes at elevated temperatures are being obtained.

Johns Hopkins University
Baltimore, Maryland 21218

227. *Ionic Aspects of Soot Formation*
W.S. Koski, Dept. of Chemistry **$68,000**

By using tandem mass spectroscopic techniques, we are studying ion-molecule reactions that are of potential importance to combustion. It is observed that reactions such as $C_2H_2^+ + C_2H_2$ and $C_2H_4^+ + C_2H_4$ form condensation products (i.e., $C_4H_4^+$ and $C_4H_8^+$ respectively) under binary collision conditions. On the other hand, the reaction $C_2H_3^+ + C_2H_2$ does not form condensation products under the same conditions, although the ion $C_4H_3^+$ is observed in flames. By running an electron bombardment ion source at high pressures, we find the $C_4H_5^+$ ion when acetylene in the source is maintained at pressures greater than 0.5 torr. Other interesting ions such as $C_4H_{11}^+$ and $C_4H_4^+$ were also observed and are being studied by collision induced dissociation methods. Helium is used as a target gas. The interesting point about these ions made in this manner is that in any one of them not all of the carbon atoms are covalently bonded, but rather they are cluster ions in which an ion is bound to a neutral molecule by a small binding energy ranging from 0.1 eV to a few Kcal/mol. The binding energies of these clusters are being measured and their properties are being investigated.

Kansas State University
Manhattan, Kansas 66506

228. *Diffusion Flame Studies of the Chemical and Physical Mechanisms of Soot Formation From Aromatic and Substituted Aromatic Fuels*
J.F. Merklin, C.M. Sorensen, Dept. of Nuclear Engineering **$60,000**

We have continued our measurements of soot particulate sizes in flames using both the extinction/scattering ratio method and Photon Correlation Spectroscopy. The feasibility studies of size distribution measurements using PCS have begun. First, we have used model size distributions to create computer generated light-scattering data. These data have been fit in three different ways to determine the relative feasibilities of size distribution determinations. Second, we have measured PCS spectra from soot in a premixed CH_4/O_2 flame. The data have been analyzed by these methods and have indicated width parameters in the range $\sigma = 1.30 - 1.35$. The same CH_4/O_2 flame was chemically sampled and the sample was analyzed for the major and minor component concentrations. These results are in substantial agreement with the results previously reported in the literature. The isomeric distribution in the C_4 hydrocarbons suggests that they are formed by the reaction of C_2 hydrocarbon radicals.

Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

229. *Aromatics Oxidation and Soot Formation in Flames*

J.B. Howard, Dept. of Chemical Engineering **$90,600**

The objective of this research is to provide basic information on the kinetics and mechanisms of aromatics oxidation and soot formation in flames. The research is based on detailed measurements of profiles of soot particle number concentration and particle size distribution and stable and radical gas species concentrations through the reaction zone of low-pressure flat premixed flames. A molecular-beam sampling instrument with on-line mass spectrometry is being used for gas species measurement. Soot particles are being studied by laser scattering and adsorption measurements in the flame and analysis of beam deposits. Net reaction rates calculated from these measurements are used in screening tests of hypothetical reaction mechanisms. The gas species profiles are used to test and to extend existing flame chemistry models. The work is expected to lead to an improved understanding of the chemistry of soot formation and aromatics reactions in flames.

230. *Depopulation Rates For Combustion-Related Species in Long-Lived (>100μs) Vibrationally or Electronically Excited Levels*

J.L. Kinsey, R.W. Field, Dept. of Chemistry **$112,000**

In this project, a new technique called Stimulated Emission Pumping (SEP) is being used to study individual levels of polyatomic molecules with chemically significant amounts (up to ~3.5eV) of vibrational excitation. Current effort focuses on the acetylene molecule, HCCH, in its electronic ground state ($X^1\Sigma g$). Individual rotation-vibration levels as much as 28000 cm^{-1} above the vibrationless level are being studied to obtain information about the transition from regular to chaotic behavior in a molecular system. Parallel investigations are probing triplet levels of acetylene at ~45000 cm^{-1}, using Zeeman quantum beat spectroscopy and anticrossing spectroscopy. Among other things, these studies address the location of the $HCCH \rightarrow H + C_2H$ dissociation limit from the variation of the density of triplet levels.

National Bureau of Standards
Washington, District of Columbia 20234

231. *Laser Studies of Chemical Dynamics at the Gas-Solid Interface*

R.R. Cavanagh, D.S. King, Center for Chemical Physics **$50,000**

This is an experimental program aimed at obtaining a detailed understanding of energy transfer and molecular dynamics occurring at the gas-surface interface. High resolution, pulsed laser techniques are used to probe the internal state distribution, molecular orientation, and state dependent angular flux and velocity distribution for free molecules which result from a variety of surface desorption processes. Current work utilizes laser excited fluorescence to probe the thermal desorption of nitric oxide from Ru(001), where the rotational state, spin-orbit state, lambda doublet species, and orientation effects are being determined. Doppler studies are being used to obtain rotational state resolved angular flux and velocity distributions. This work is being extended to include a variety of thermal heating rates of the surface and a study of the influence of different substrates, such as Pt(111) and Pd(111).

232. *Kinetics Data Base For Combustion Modeling*

W. Tsang, R.F. Hampson, Center for Chemical Physics **$63,000**

The aim of this research is to compile, evaluate, and publish information on the rate constants for single step chemical processes which are pertinent to the detailed description of hydrocarbon combustion processes. The plan of attack is to start with the simplest molecular systems, and then to expand into more complicated situations. All possible reactions are considered. Evaluation involves critical examination of experimental data, comparisons with analogous reactions, and expectations from theory. Where data do not exist, estimates are made. Results are presented on individual data sheets so as to permit periodic upgrading. Work on methane and ethane oxidation and pyrolysis have been completed. It should be noted that these reactions form a subset of all combustion processes. Further work will involve continuous updating and expansion into NO_x, CH_3OH, and higher hydrocarbon systems.

Princeton University
Princeton, New Jersey 08544

233. *Comprehensive Mechanism For Combustion Chemistry: An Experimental and Numerical Study With Emphasis on Applied Sensitivity Analysis*

F.L. Dryer, Dept. of Mechanical and Aerospace Engineering **$90,000**

This program is an integrated effort to determine the reaction mechanisms responsible for oxidation of hydrocarbon and alcohol molecular structures under conditions representative of combustion environments. Such mechanisms are useful to focus on areas where further elementary processes research would be most beneficial, in acting as bench marks against which simplified empirical chemistry results can be compared, and in evaluating the interactions of combustion chemistry within simple one-dimensional, time transient systems with transport. The program necessitates a three-pronged approach: (1) experimental effort for determining pyrolysis and oxidation intermediate and product profiles in a turbulent flow reactor; (2) comprehensive mechanism development and accompanying computer modeling; and (3) application of newly available sensitivity analysis computer tools to extract the maximum information from the first two parts of the research. Efforts are coordinated with the sensitivity analysis research of Rabitz at Princeton, the modeling efforts of Westbrook at Lawrence Livermore National Laboratory, and the fundamental kinetics program of Klemm and Michael at Brookhaven National Laboratory. The experimental aspects of the program are conducted in a flow reactor facility developed at Princeton which permits chemical kinetic observations at atmospheric pressure, in the temperature range of about 900 K to 1200 K, and for reaction times the order of 10 to 500 msec. The modeling aspects of the program are accomplished through use of several recently available computational tools (e.g., HCT, AIM, and CHEMSEN) and other tools and techniques as they become available. Chemical systems of current interest (in order of increasing complexity) are:

the $CO/H_2/O_2$ system, the formaldehyde pyrolysis and oxidation systems, the acetaldehyde pyrolysis and oxidation systems, and the ethanol pyrolyis and oxidation systems.

234. *Dynamical Studies of Molecular Systems*

H.A. Rabitz, Dept. of Chemistry **$134,000**

The research project has two parts consisting of studies in chemical kinetics and collision dynamics. In the first part on chemical kinetics, the research is concerned with the development and application of sensitivity analysis tools for the understanding of complex chemical mechanisms. Both time and spatially dependent problems are under study with a special emphasis on combustion phenomena. In the latter case, sensitivity techniques are being developed for probing the role of rate constants, transport coefficients, initial conditions, and boundary conditions on laboratory observables. The second part of the research in collision dynamics is concerned with phase space trajectory analysis and the development of collisional scaling relationships. Scaling has the goal of providing the theoretical framework for taking laboratory data to a more fundamental underlying level, such that it may be used again to produce new observable collision phenomena. A hierarchial approach to the theory of collisional scaling is being taken whereby the scaling relations may be employed with various levels of sophistication. Finally, a theory for the structural analysis of classical phase space trajectories is being developed. The approach allows for the calculation of a small number of structural constants which physically characterize the shape of the trajectory.

Purdue University
West Lafayette, Indiana 47907

235. *Measurement of Radical Species Concentrations and Polycyclic Aromatic Hydrocarbon in Flames By Fluorescence and Absorption Via Tunable Dye Laser*

N.M. Laurendeau, Dept. of Mechanical Engineering **$94,000**

New quantitative laser fluorescence techniques are being developed to measure the concentrations of radical species and polycyclic aromatic hydrocarbons (PAH) in flames. Previously we have: (1) demonstrated laser-saturated fluorescence (LSF) measurements of OH and NH concentrations using a flat flame burner operated under a variety of flame pressures, temperatures, and equivalence ratios; (2) developed a potential technique for determining PAH concentrations in a vapor mixture; and (3) made the first reported fluorescence measurements of atomic hydrogen in flames using two-photon absorption. Recently, we have improved the calibration procedure and investigated the effects of non-uniform laser illumination for the LSF measurements. Current research includes: (1) laser-saturated CN and CH measurements; (2) PAH measurements using one- and two-photon excitation; and (3) two-photon measurements of atomic hydrogen and oxygen in flames.

Rensselaer Polytechnic Institute
Troy, New York 12181

236. *Kinetic Measurements On Elementary Fossil Fuel Combustion Reactions Over Wide Temperature Renges*

A. Fontijn, Dept. of Chemical & Environmental Engineering **$85,000**

This research project is aimed at providing kinetic data on important isolated elementary hydrocarbon molecule oxidation reactions. Emphasis is placed on measurements in the 1000-1800 K range, where accurate data are generally not available, but needed for development of improved fossil-fuel utilization methods. The high-temperature photochemistry (HTP) adaptation of the flash-photolysis resonance-fluorescense technique is further developed. Use is made of fast electronics, which allows rapid data taking and short residence times and of on-line microcomputer data smoothing procedures which minimize the number of flashes required. The first objects for study are reactions between O atoms and C_2 hydrocarbons.

Rice University
Houston, Texas 77251

237. *Infrared Absorption Spectroscopy With Color Center Lasers*

R.F. Curl, Jr., Dept. of Chemistry **$65,000**

This research project is directed at the development of high sensitivity, high resolution methods for detecting and monitoring small free radical species which are thought to be important intermediates in combustion by means of infrared absorption spectroscopy using color center laser sources. Two new high sensitivity spectroscopic methods which can be combined with the long pathlengths obtainable with a White cell have been developed. One, a magnetic rotation technique for the suppression of source noise, provides a high sensitivity absorption spectroscopy which is selective for free radicals. The other, a high sensitivity spectroscopic method suitable for non-magnetic molecules, uses electro-optic tone modulation of the color center laser infrared output. For the latter technique, a CdTe electro-optic modulator was specially designed and has recently been successfully tested. Earlier, the magnetic rotation method was used to observe and assign the electronic spectrum of C_2H in a discharge through argon over polyacetylene. In the continuation of this work, efforts will focus upon the identification of other radical species present in the discharge over polyacetylene as evidenced by as yet unassigned Q-branches. When observed by the tone modulation technique, the entire structure of these band fragments should be revealed.

238. *Supersonic Metal Cluster Beams*

R.E. Smalley, Dept. of Chemistry **$75,000**

Laser vaporization of a metal target within a pulsed supersonic nozzle is used in this research to prepare beams of transition metal clusters. This new technique (developed in the previous year of this DOE contract) is perfectly general for even the most refractory metals (e.g., tungsten), and readily provides an intense source of bare metal clusters cooled to internal temperatures on the order of 5 K. Current research with this new source centers around the spectral study of small transition metal clusters, in order to obtain accurate and definitive measurements of the metal-metal bond (bond length, dissociation energy, electronic structure, bond angles, vibrational frequencies, etc.). Metal clusters studied thus far include Cr_2, V_2, Ni_2, Cu_2, Cu_3, and Mo_2. The results in the case of Cr_2 and V_2 indicate that the metal-metal bond in this region of the transition series is dominated by strong 3d orbital interaction, resulting in extremely short bond lengths. Nickel and copper, on the other hand, are found to be bound mostly through the 4s orbitals.

SRI International
Menlo Park, California 94025

239. ***Combustion Research Program: Flame Studies, Laser Diagnostics, and Chemical Kinetics***
D.R. Crosley, Molecular Physics Lab **$114,900**

This research project involves a combination of laser-induced fluorescence (LIF) and chemical kinetics measurements to investigate the chemistry of hydrocarbon and ammonia combustion processes. The research comprises several related parts: (1) LIF probing of flat flames; (2) the development of an LIF spectroscopic and collisional data base; (3) computer modeling of combustion chemical networks; (4) development and application of rate constant estimation methods; and (5) a laser pyrolysis (LP)/LIF experiment. In LP/LIF, a mixture containing SF_6 is rapidly heated by a pulsed CO_2 laser, with time-resolved LIF measurements of radical concentrations and temperature. Measurements of the $OH + C_2H_2$ rate constant show an abstraction (addition) mechanism dominating above (below) 1000 K, agreeing with theoretical calculations of the combined pressure/temperature dependence of the addition channel. LP/LIF measurements on $OH + CH_4$, C_3H_8, C_3H_6, and NH_3 have also been made. Calculations on the $H + N_2O$ reaction and $CH_3 + CH_3$ recombination show bound intermediates and very different rate constant expressions from those currently used. The LIF spectroscopy of the $A^3\Pi_i$-$X^3\Sigma^-$ system of NH in a flow system has yielded lifetimes and transition probabilities, and the LIF flame spectra of NH_2 in $NH_3/O_2/N_2O$ flames is being catalogued.

Stanford University
Stanford, California 94305

240. ***Studies of Combustion Gas Spectroscopy Using Tunable Lasers***
R.K. Hanson, Dept. of Mechanical Engineering **$55,000**

Objectives of this research are: (1) the measurement of fundamental spectroscopic parameters (absorption coefficients, band or oscillator strengths, and collision widths) for critical combustion species, particularly pollutants and radicals; and (2) the development of tunable laser absorption and fluorescence techniques for species measurements in studies of chemical kinetics. Laser sources include a tunable CW infrared diode laser, a tunable CW ring dye laser, and a discretely tunable CO laser. Species studied include HCN, CO, OH, NH, CH, NCO, and water vapor. Measurements are made over a range of conditions in a controlled-temperature absorption cell, in the post-flame region of a flat flame burner, and in a shock tube.

241. ***The Kinetics of Some Reactions of HCN At High Temperature***
R.K. Hanson, C.T. Bowman, Dept. of Mechanical Engineering **$70,000**

The objective of this research project is to obtain high-temperature kinetic data for reactions involving HCN and the CN radical. These data are relevant to the formulation of reaction mechanisms for pollutant formation in flames. Reactions of interest include: (1) the thermal decomposition of HCN, and the reactions of HCN with CN, H, O, and OH; (2) the thermal decomposition of C_2N_2; and (3) the reactions of CN with O and O_2. A conventional shock tube technique is combined with spectroscopic diagnostics to study the mechanisms and rates of candidate reactions. Experimental data are compared with results obtained from empirical models.

State University of New York/Buffalo
Amherst, New York 14226

242. ***Multiphoton Interactions in Molecules With Picosecond Laser Pulses***
H.S. Kwok, Dept. of Electrical and Computer Engineering **$64,000**

High power CO_2 laser pulses are employed in this research program to study the multiphoton behavior of polyatomic molecules. During the past year, we have carefully measured the excitation of SF_6 by picosecond laser pulses with various durations. A second laser was added to the experimental setup to preheat the SF_6 molecules into the quasicontinuum of vibrational states. It was found that the multiphoton excitation depended only on the intensity of the laser pulse, for durations between 38 and 150 ps. This indicates a breakdown of the energy fluence scaling law and points directly to coherent excitation in the quasicontinuum. It is first firm experimental evidence of coherent excitation of any system in the presence of strong intramolecular damping. We have developed an N-level Bloch equation model that includes both coherent and incoherent excitation in the quasicontinuum. The experimental data are commensurate with slow intramolecular energy transfer and increasing oscillator strength as the molecular is excited. Other molecules will be tested using the same techniques.

State University of New York/Stony Brook
Stony Brook, New York 11794

243. ***Multiphoton Ionization Spectroscopy and Photochemistry of Transient Species***
P.M. Johnson, Dept. of Chemistry **$65,000**

This project is primarily concerned with the development of new methods of acquiring the multiphoton spectra of transient species such as triplet metastables and radicals. These species are generated in ways which are related to combustion processes so that insight may also be gained into the production mechanisms. In one method, radicals and triplets are generated by a pulsed electric discharge at the orifice of a pulsed supersonic valve, providing cooling in the expansion and a rapid transition into a collisionless condition. This technique has proven to be a bountiful source of triplet and radical species whose multiphoton spectra have never been explored. It should also be possible to create discharge initiated reactions between two species in the expansion. Reaction intermediates will be rapidly isolated by the expansion and can be studied by multiphoton ionization mass spectrometry. To date, we have successfully studied the triplet states of argon, carbon monoxide, and benzene as well as the radical CCl.

University of Arizona
Tucson, Arizona 85721

244. *Experimental Studies of the Ionizations and Bonding of Small Molecules Attached to Transition Metals*

D.L. Lichtenberger, Dept. of Chemistry **$77,000**

This research project focuses on experimental investigation of the electronic mechanisms of bond activation of small molecules by transition metals. The primary experimental technique is gas-phase photoelectron spectroscopy, utilizing HeI, HeII, and X-ray excitation sources. Breakthroughs have been made with the HeI source in observing detailed vibrational structure in metal ionizations. An improved HeII source design has proven to be especially valuable in understanding the valence ionizations of organometallic molecules. Gas phase core photoelectron spectroscopy has been developed, and has shown important correlations between core and valence ionizations shifts. The systems receiving most attention involve metal interactions with small organic species that are proposed intermediates in water-gas shift and Fischer-Tropsch catalysis, such as alkyls, alkenes, alkynes, methylenes, and vinylidenes. An important new study involves investigation of metal-alkyl complexes that represent intermediate stages of carbon-hydrogen bond breaking and formation. We have also recently acquired new state-of-the-art instrumentation for applying these photoelectron techniques to the study of molecules on surfaces. This will allow development of a more complete relationship with surface chemistry and catalysis.

University of California/San Diego
La Jolla, California 92093

245. *Shock-Tube Studies of Important Combustion-Reaction Steps Involving Radicals*

K.G.P. Sulzmann, Energy Center **$63,500**

The aim of this research is twofold: (1) the use of shock-tube techniques for the rapid introduction of known intermediate and radical concentrations into a combustion environment, in which the individual interactions of these species with other reactants and intermediates can be separated or enhanced for meaningful rate measurements of individual or sub-groups of reaction paths relevant to hydrocarbon combustion; and (2) the use of *in situ* quantitative spectroscopic measurement techniques, for the determination of required species concentration-time histories. As a first step, the only partly understood fate and kinetics of the CH_3-radical is investigated during its donor-pyrolysis, and its interactions with O_2 and O-atoms behind reflected shock-waves by using argon-diluted $CH_3CO_2CH_3$, $(CH_3)_2$, CH_3COCH_3 and /or CH_3N_2 as methyl radical donors. Oxidation reactions are initiated by admixing either O_2 or N_2O as an O-atom donor. Quantitative spectroscopic data are obtained by infrared emission (2 channels), by infrared HeXe-laser absorption at 3.508μ, by visible ultraviolet emission (10 channels), and/or by vacuum-ultraviolet absorption.

University of Chicago
Chicago, Illinois 60637

246. *Topics in Finite Time Thermodynamics*

R.S. Berry, James Franck Institute **$72,000**

The term "finite time thermodynamics" refers to the extension of traditional thermodynamics to the description of systems and processes whose constraints include finite times or nonzero rates of operation. In particular, the term refers to the determination of the extremal performance and the paths that would yield that performance, when the constraints of finite-time operation must be met. The progress of this group since the last report has included: (1) the theoretical description and elaboration of a new type of engine, based on a dissipative progress; (2) an analysis of space heating under periodic illumination conditions (as with the diurnal variations of solar systems), with control by (nonenergy-consuming) variation of insulation; an analysis of the entropy production by such a system; (3) the exploration of geometric formulation of thermodynamics based on the metric introduced by Weinhold, including the proofs of relations between dissipation in a finite-time process and the "length" of the path for that process calculated by Weinhold's metric; and (4) the further extension of the concept of availablilty (exergy) to processes operating in finite time, and the application of this extended concept to extraction of work from a system not initially in internal equilibrium.

247. *Laser Induced Chemical Reactions and Laser-Collision Processes*

J.C. Light, James Franck Institute **$70,000**

Laser induced chemical processes of several types have been observed experimentally. Our research program is to develop theoretical methods to examine some of these and related processes. Methods to do exact 3-D quantum calculations of single photon photodissociation of triatomic molecules have been developed and applied to models of HCN and ICN. A new representation of the problem (discrete variable representation) simplifies the calculation considerably by taking advantage of the localization of the initial state. These techniques are now being applied to the related problems of dissociative attachment in electron molecule collisions ($e^- + F_2$, $e^- + CO_2$) and to dissociation by photoemission from Rydberg states H_3^*(Rydberg) $\rightarrow H_2 + H + h\nu$. Realistic calculations of multiphoton dissociation of O_3 in intense laser fields are being done using a realistic internal state structure and our recently developed rotating frame transformation.

University of Colorado
Boulder, Colorado 80309

248. *Laser Photoelectron Spectroscopy Of Ions*

G.B. Ellison, Dept. of Chemistry **$165,000**
(18 mo.)

Laser photoelectron spectroscopy has been used to study a number of simple negative ions. Our experiments produce direct, reliable thermodynamic information such as electron affinities, radical and ion heats of formation, and bond dissociation energies. These are crucial data required for an understanding of combustion processes. We have completed careful studies of HNO^-, DNO^-, CH_2CCH^-, CH_2CCD^-, CD_2CCH^-, CCO^-, $HCCO^-$, and $DCCO^-$. We have just finished work on CH_2CN^-,

CD_2CN^-, CH_2NC^-, and CH_3CHCN^-. Proposed research centers on polymeric carbon ions (C_n^-), allyl anion ($CH_2=CH\text{-}CH_2^-$), and CO_2^-.

249. *Time-Resolved Studies of Free Radicals and Laser-Initiated Chain Reactions*
S.R. Leone, Dept. of Chemistry **$70,000**

Time and wavelength-resolved infrared emission techniques are used to study free radical production and reactions. Infrared emission spectra have been obtained and analyzed for combusting mixtures of low-pressure chlorine with hydrocarbons. A method has been developed to measure the absolute rate coefficients of methyl radical reactions with molecules such as chlorine, bromine, and hydrogen iodide. Intramolecular vibrational relaxation processes have been observed in the ground electronic state of hydrocarbons by exciting the first CH overtones and detecting the reduction in emission from these states. A multiple vibrational state analysis has been developed and applied to the extraction of rate information for very slow chain reactions.

University of Illinois
Chicago, Illinois 60680

250. *Kinetics of Elementary Atom and Radical Reactions*
R.J. Gordon, Dept. of Chemistry **$70,700**

The objectives of this research are to measure the reaction rates and to study the dynamics of elementary gas phase reactions, using sensitive, real time techniques to eliminate systematic errors. One system being studied is $O + H_2$, D_2 and HD. Flash photolysis with resonance fluorescence detection of oxygen atoms has been used to measure the rate constants of these reactions between 325 and 475 K. The intramolecular branching ratio for O + HD is being determined by using laser-induced fluorescence to measure the relative concentrations of OH and OD products. In a separate study, the relaxation of highly excited molecules is being studied by using a CO_2 laser to excite a donor molecule while detecting IR fluorescence from a receptor molecule. Studies of $SF_6 + N_2O$ and SF_6 + NO yield the VV transfer rate as a function of SF_6 excitation. The observation of a slower decay rate at higher excitation levels indicates the existence of an energy storage mechanism in the SF_6 molecule.

251. *Laser Schlieren, Shock Tube Studies of High Temperature Hydrocarbon Pyrolysis Rates*
J.H. Kiefer, Dept. of Chemical Engineering **$65,000**

This project investigates the rates and mechanism of fuel pyrolysis reactions of importance in combustion at very high temperatures. Experiments use the shock tube in conjunction with laser-schlieren diagnostics capable of providing an accurate measure of initiation rates with 0.1 μs resolution as well as some secondary rates. Rates and mechanisms for the pyrolysis of propane, propene, ethane, ethylene/acetylene, butadiene, benzene, and toluene have been investigated. The ethane study strongly indicates that methyl-methyl reactions, other than recombination, do not occur at significant rates to 2700K. The butadiene study suggests a low heat of formation for vinyl radical ($\Delta H_{f,298}^\circ < 65$ kcal/mole), and an estimate for the high-T vinyl radical dissociation rate, a rate of considerable importance in combustion modeling.

University of Kansas
Lawrence, Kansas 66045

252. *Molecular Design Principles For Biomimetic Solar Energy Conversion Systems*
G.M. Maggiora, Dept. of Biochemistry **$89,400**

Ab initio quantum mechanical and empirical potential function procedures are being applied in an investigation of the physicochemical factors underlying biological and biomimetic solar energy conversion, and these factors will be used to develop a set of molecular design principles, which will enable chemists to formulate structures of potential biomimetic photoconversion systems possessing specified properties more efficiently. Current studies are directed towards porphyrin dimer and trimer systems, especially hetero-dimers. Preliminary results indicate the existence of low-lying, non-radiative charge-transfer states in magnesium porphine-porphine dimers which may be sufficiently long-lived to facilitate electron transfer from these dimers to appropriate acceptors. The results are being futher evaluated with regard to the effects of intermolecular geometry and microenvironment on the location and character of the charge-transfer states. Studies are also continuing on the evaluation of possible molecular candidates for the P700 and P680 photoactive species in the photoreaction centers of green plants. In addition, the development of new and improved theoretical methodologies and algorithms are being actively pursued.

University of Minnesota
Minneapolis, Minnesota 55455

253. *State-to-State Dynamics of Molecular Energy Transfer*
W.R. Gentry, C.F. Giese, Depts. of Chemistry and Physics **$80,000**

A novel pulsed molecular beam instrument has been constructed for the study of state-to-state vibrational and rotational energy transfer in collisions of atoms and molecules. The results are expected to lead to an understanding of molecular energy transfer on a microscopic level, including the dependence of energy transfer processes on the vibrational and translational energies of the colliding molecules. The first experiments measured the kinetic energy dependence of the vibrational excitation cross sections for I_2 + He collisions. Similar measurements have now been performed for $I_2 + D_2$ and I_2 + Ne collisions, in order to explore the effects of mass and features of the potential energy surface on the excitation dynamics. These experiments are being extended to other systems, including mode-specific excitation of the polyatomic molecules aniline and p-difluorobenzene.

254. *Variational Transition State Theory*
D.G. Truhlar, Dept. of Chemistry **$70,000**

This research project is an attempt to develop and implement new methods for calculating rate coeffecients for chemical reactions from potential energy surfaces. Emphasis is being placed on gas-phase atom-transfer reactions, which are an important reaction type in combustion and atmospheric systems, as well as being of fundamental interest. We are also studying the effect of vibrational excitation of the reactants on chemical reaction rates, and we are studying kinetic isotope effects. A very important aspect of our studies is the inclusion of quantal effects in reaction rate calculations, with special emphasis on tunneling (barrier penetration), and on the dependence of vibrational frequencies on the reaction coordinate. We are developing methods to model the potential energy surfaces for simple reactions and also to utilize *ab initio* reaction-path Hamiltonians in our calculations. Examples of our applications to reactions important in combustion are $OH + H_2 \rightarrow H_2O + H$, and $OH + O \rightarrow H + O_2$, and $O + H_2 \rightarrow OH + H$.

University of New Orleans
New Orleans, Louisiana 70148

255. *Identification and Temporal Behavior of Radical Intermediates Formed During the Combustion and Pyrolysis of Gaseous Fuels*

R.D. Jr. Kern, Dept. of Chemistry **$60,000**

The practical and environmentally acceptable use of fossil fuels containing aromatic hydrocarbons in furnaces and engines is dependent upon the control of soot formation. The chemical sequence of reactions which lead to soot are being investigated by recording the product profiles generated during the pyrolyses of toluene, benzene, allene, butadiene, and acetylene. The experimental technique utilized involves the dynamic sampling of the reflected shock zone by time-of-flight mass spectrometry. Data have been obtained over a wide range of temperature and fuel concentrations. Computer modeling has successfully fit many of the experimental profiles. The major findings are: (1) the dominance of the ring fragmentation routes as opposed to ring condensation steps in the pyrolyses of toluene and benzene; (2) the limited amount of ring formation observed in the decompositions of allene and butadiene; and (3) the absence of ring species formed during the polymerization of acetylene.

University of Rochester
Rochester, New York 14627

256. *Low Energy Ion-Molecule Reactions and Chemiionization Kinetics*

J.M. Farrar, Dept. of Chemistry **$70,000**

Molecular beam reactive scattering measurements of proton transfer reactions of the flame cations HCO^+ and H_3O^+ with neutral molecules present in hydrocarbon flames are being carried out to understand the dynamics of ionic processes occurring in flames. Measurements of product angular and kinetic energy distributions yield energy disposal in reactive collisions, inferences concerning preferred collision geometries, and in favorable cases, determination of specific quantum states of nascent reaction products. Proton transfer reactions to the substrates H_2O, CH_3OH, C_2H_5OH, and $(CH_3)_2C{=}O$ have been studied, indicating direct reaction dynamics. Unimolecular decay channels of protonated products are studied and decays involving bond cleavage, 1,3-hydrogen atom shifts, and elimination of molecular hydrogen across the C-O bond have been observed. In the latter case, variations of proton donor modifies the parent ion internal state distribution; such observations are being employed to assess the role of tunneling through the exit channel barrier in the elimination process. Work in progress involves hydride transfer reactions of CH_3^+ as well as studies of carbon cations, C^+, with small hydrocarbons.

University of Utah
Salt Lake City, Utah 84112

257. *Study of Combustion and Flame Processes Initiated By IR Laser-Induced Absorption*

W.A. Guillory, Dept. of Chemistry **$80,000**

The phenomenon of infrared multiple-photon absorption (IR MPO), subsequently leading to excited and ground state dissociation products, simulates non-equilibrium processes occurring in flames and other combustion systems. Using visible and UV laser-induced fluorescence diagnostics as probes of the reaction zone, highly sensitive time and wavelength resolved spectroscopy allow detailed determination of the mechanisms and energetics of a given system. The reactions of vibrationally excited ground electronic state CH and OH (produced by IR MPO) with O_2, N_2, NO, and aliphatic and aromatic hydrocarbons are being studied. Also being studied is the efficiency and means of production, via IR MPO, of CH and OH from various precursors. New techniques, such as multi-photon absorption fluorescence, are being implemented to study amounts of and energy states of reactive and product species (CH_2, CH_3, C, and so forth). Discrete level and quasicontinuum energy transfer and relaxation in propynal, glyoxal, and methylglyoxal are also being studied.

University of Wisconsin
Madison, Wisconsin 53706

258. *Unimolecular Reaction Dynamics*

F.F. Crim, Dept. of Chemistry **$52,400**

This program is an experimental study of the unimolecular decay dynamics of internal energy selected molecules using direct production of highly vibrationally excited molecules by dye laser excitation of overtone vibrations in conjunction with time resolved spectroscopic detection. Excitation of an overtone vibration prepares a molecule with a large excess of energy initially isolated in a small subset of the available vibrational modes. Time-resolved spectroscopic detection provides a direct measure of the unimolecular reaction rate constant and, in favorable cases, the energy partitioning in the products. This work includes excitation of both CH and OH overtone vibrations and product detection using both visible chemiluminescence and laser induced fluorescence. The most extensive recent results are on hydrogen peroxide (HOOH) and its partially deuterated analogue (HOOD) initially excited with five ($5\nu_{OH}$) or six ($6\nu_{OH}$) quanta of stretching in the OH bond. These detailed studies critically test statistical theories of unimolecular reactions and provide data on the dynamics of isolated molecules which are potentially useful in understanding atmospheric chemistry, combustion processes, and laser induced reactions.

Wright State University
Dayton, Ohio 45435

259. *Direct Determination of Atom and Radical Concentrations in Thermal Reactions of Hydrocarbons and Other Gases*

G.B. Skinner, Dept. of Chemistry **$58,400**

The general goal of this research is to study the kinetics of the atom and free radical reactions that are important in combustion reactions by following the appearance and disappearance of H, O, OH, and other such combustion intermediates. H, D, and O atoms are currently being measured in shock tube experiments using resonance adsorption spectroscopy in the vacuum ultraviolet. Measurements made recently involve pyrolysis of butadiene, and analysis for both H and D in pyrolysis of partially deuterated propene. A series of experiments in which H Atoms produced by dissociation of neopentane or toluene react with acetylene-d_2 has been carried out to study the formation and stability of the vinyl radical. Measurements of both H and D concentrations help to clarify the reaction mechanisms. The shock tube has recently been modified to extend the range of total pressures from 3 atmospheres down to 0.4 atmospheres, so the dependence of reactions on total pressure can be more effectively studied.

Yale University
New Haven, Connecticut 06520

260. Simultaneous Multipoint Measurements of Density Gradients and Temperature in a Flame
R.K. Chang, B.T. Chu, M.B. Long, **$68,000**
Section of Applied Physics and
Dept. of Mechanical Engineering

The main thrust of this research program is directed toward developing new *in situ* optical techniques for characterizing turbulent reactive and nonreactive flows. Central to the technique developed in mapping two-dimensional concentration distributions in such flows is the use of a low-light-level television camera capable of detecting the scattered radiation from 10^4 discrete volumes in the flow. Such measurements, while instantaneous, can be recorded only at ~30 frames/s which is too slow to follow the temporal evolution of turbulent structures and flame sheets. We have recently succeeded in increasing the effective frame rate of our existing slow camera 70-fold to ~2000 frames/s by inserting a rotating mirror in our detection system and synchronizing the laser pulse rate with the rotational velocity of the mirror. Further increase of the effective frame rate is being explored. In another study, we have demonstrated that broadband rotational CARS is a potentially viable technique for single-pulse flame temperature measurements and that simultaneous temperature and species measurements with rotational CARS from many spatially resolved volume elements along a cylindrical line in room-temperature gases are feasible.

Atomic Physics

Atlanta University
Atlanta, Georgia 30314

261. Theoretical Investigation of Electron-Ion Interaction
A.Z. Msezane, Dept. of Physics **$50,000**

The purpose of this project is to identify and calculate dominant physical mechanisms underlying the processes of electron impact excitation and ionization of ions using the close-coupling approximation. Both total and differential cross sections are calculated and compared with measurements. In particular, detailed numerical studies are carried out to investigate the extent of contribution of the physical processes of inner-shell excitation- autoionization and inner-shell resonant-excitation-double autoionization to the total ionization cross section of Ti^{+3}, important in CTR plasmas. Also, total and differential cross sections for electron impact excitation of Cd II, important in the He - Cd II Hollow-cathode laser, are compared with measurements from energy loss spectrum and line emission data. An accurate configuration-interaction wave function of the target is used, to give the energy splittings between the ground state and the various excited states of interest very close to the observed values, and the same values for the oscillator strengths in the length and velocity formulations.

College of William and Mary
Williamsburg, Virginia 23185

262. Collisional Detachment of Negative Ions
R.L. Champion, L.D. Doverspike, **$80,000**
Dept. of Physics

The fundamental goals of these experimental studies are to determine various cross sections, and to develop a general understanding of the collisional dynamics for systems which involve negative ions. The energy range of the experiments is from a few electron volts up to 500 eV. The experiments involve measurements of absolute total cross sections and doubly-differential cross sections. The processes under investigation include collisional detachment, charge transfer, dissociative charge transfer, reactive scattering, and inelastic scattering. Emphasis is placed upon developing an understanding of the role of competing product channels in negative ion-molecule collisions and upon delineating the various collisional processes that may occur in collisions of negative ions with molecular targets. Systems which are being investigated include hydrogen, deuterium, oxygen and halogen negative ions in collisions with hydrogen, deuterium, halogen molecules, O_2, HCL, N_2, CO, CO_2, and CH_4. The experimental results are coupled with theoretical models to provide a basis for understanding the role of negative ions in various environments.

Cornell University
Ithaca, New York 14853

263. Experimental Study of Interactions of Highly Charged Ions With Atoms At keV Energies
V.O. Kostroun, Nuclear Science **$180,000**
and Engineering Program

Experimental and theoretical interest in interactions of low energy highly charged ions with atoms or ions is due to the relevance of such interactions to controlled thermonuclear fusion research and to the interesting nature of the fundamental processes involved. This program centers around experimental investigations of interactions of highly charged ions and atoms at low energies, and consists of two parts. One involves atomic physics experiments and source studies and development using a small electron beam ion source (EBIS) called CEBIS I. The other, initiated in August 1983, involves the design, construction, and development of a larger superconducting solenoid version called CEBIS II. CEBIS I is used to investigate low energy charge transfer to multiply charged ions, in particular to measure partial cross sections for population of specific states of the projectile as a function of its energy for C^{q+}, N^{q+} and O^{q+} ($q \geq 3$) colliding with molecular hydrogen and helium in the 0.05

qkeV to 5 qkeV range. Specific states of the projectile populated in the collisions are selected by high resolution energy gain spectroscopy. The immediate goal of CEBIS II will be to generate a usable, ~ 3 qkeV beam of Ar^{18+}. Longer range goals include optimization of the source and gradually upgrading it to handle a 25 kV, 1 A electron beam which could be used to produce He-like xenon.

Harvard University
Cambridge, Massachusetts 02138

264. *Theoretical Studies of Highly Ionized Species*
A. Dalgarno, Harvard-Smithsonian Center For Astrophysics **$130,000**

Studies are made of collisions of multiply-charged ions with neutral gas affect the ionization structure, thermal balance, radiation losses, and ion transport in plasmas containing a neutral component. Because the products of the collisions radiate, they can be detected and thereby provide unique diagnostic probes of the environment. We have extended our calculations of the efficiencies of the processes so that their accuracy can be assessed by comparison with experimental data, which are now becoming available. We have made estimates of charge transfer into individual fine-structure states because observations of astrophysical objects show that the separate emission lines can be distinguished readily. We have also explored collisions of positive and negative ions.

Jackson State University
Jackson, Mississippi 39217

265. *Spectroscopy of Trapped Molecular Ions*
J. Perkins, G. Miller, Dept. of Chemistry **$55,000**

The goal of this project is to provide spectroscopic data that will document those characteristics of molecular ions responsible for the large cross sections accompanying ion-molecule reactions. Using laser induced fluorescence (LIF), energy level and lifetime measurements are made of various small molecular ions (e.g., O_2^+, CO^+, CH^+, and CH_2^+). The ions are prepared by fragmentation of parent neutral gases through electron impact using a Pierce-type pulsed electron gun. The ions are mass selected by, and trapped in, a quadrapole ion trap long enough to carry out the spectroscopic measurements. Attempts are made to study intramolecular and intermolecular energy exchange involving electronic, vibrational, and rotational motions of these ions. Light intensity measurements are made using a dye laser, and the results are used to determine excited state lifetimes in the order of tens of milliseconds.

Kansas State University
Manhattan, Kansas 66506

266. *Atomic Physics of Strongly Correlated Systems*
C.-D. Lin, Dept. of Physics **$86,000**

This project is directed toward the understanding of correlations of two-electron atoms in hyperspherical coordinates, and the development of practical codes for computing inelastic cross sections in ion-atom collisions. A complete classification scheme for doubly excited states is being developed. Dipole selection rules for photoabsorption are being investigated. The modified atomic-orbital model (AO+) and the triple center AO expansion method are generalized to include excitation, charge transfer, and ionization processes for calculating inelastic ion-atom collisions at intermediate and low velocities.

267. *Atomic Physics With Highly Charged Ions*
P. Richard, Dept. of Physics **$530,000**

High velocity, highly charged ions produced by the 6 MV KSU tandem Van de Graaff are used to study charge transfer, ionization, and excitation in ion-atom collisions. Electron capture by highly-charged ions, produced as recoils from fast-ion bombardment of gases is studied at very low projectile velocities. During this contract year, electron capture from lithium by very low-energy protons and helium ions has been studied. Energy-gain spectroscopy has been performed for slow, highly charged projectiles on rare gas targets. Cross sections for electron capture by similar projectiles from an atomic hydrogen target han been carried out. The production of short-lived mulitiply-charged molecular species from a recoil source has been studied. Electron capture by fast K-vacancy-bearing metastable projectiles from rare gas targets has been studied. Investigation of quasiresonant K-vacancy transfer has been extended downward in velocity revealing informative further structure in the impact-parameter dependence of the process. The Thomas peak in the angular distribution of electron-capturing protons from molecular hydrogen was observed and theoretical work completed for a quantitative understanding of the effect.

Louisiana State University
Baton Rouge, Louisiana 70803-4001

268. *Electron Collisions With Positive Ions*
R.J.W. Henry, Dept. of Physics and Astronomy **$57,000**

The fundamental goal of this project is to delineate the important physical processes which govern electron impact excitation processes for impurity ions in high temperature plasmas of interest in the thermonuclear reactors. The energy range considered is from the threshold to approximately four times the ionization energy. Calculations are based on a close-coupling expansion which includes the important physical effects of electron exchange and resonances. Calculations are made for inner-shell excitation-autoionization contributions to total ionization for Ti^{+3} and are in good agreement with known measurements. Differential electron scattering cross sections for inelastic excitation of Zn^+ are calculated at energies between 15eV and 100eV. Agreement of theory with experiment at 75eV is excellent over the measured angular range of 4° to 16°. Inelastic electron impact cross sections are calculated for Mg^+ and Al^{++}. Calculations give good agreement with recent measurements from crossed-beam experiments.

National Bureau of Standards
Washington, District of Columbia 20234

269. *Electron-Atom Collision Studies Using Optically State Selected Beams*
R.J. Celotta, M.H. Kelley, Division of Radiation Physics **$62,000**

Coherence and correlation techniques in atomic collision experiments are being used to improve our understanding of the interactions important in the atomic collision process. Production and detection of spin polarization in free electron beams and laser optical pumping methods for the production of polarized atomic beams have been used to study electron-atom collisions using quantum state selected beams. Such studies provide the maximum allowable information about the interaction, and require an experimental arrangement only slightly more complicated than a conventional crossed beam scattering apparatus. A scattering apparatus which uses optically selected beams capable of very general studies of collisions between spin polarized electrons and spin polarized atoms has been constructed. This facility will be used to make a comprehensive study of the role played by electron spin in electron-atom interactions. In particular, for alkali atoms, the exchange interaction and the spin-orbit interaction in elastic, inelastic, and superelastic collisions will be examined. The studies of electron correlation in ionizing collisions near threshold will be continued.

270. *Atomic and Molecular Collision Processes*

D.W. Norcross, Quantum Physics Division **$93,000**

The focus of this project is the physics of low energy collisions of electrons with atoms, ions, and molecules, with an emphasis on detailed computational studies. High precision calculations for elastic scattering by neutral helium are being extended to near-threshold excitation. Work on electron-impact excitation of He-like ions was extended to Ca^{+18}. All important physics (close-coupling, target fine-structure, autoionization, dielectronic recombination) is included. A new parameter-free correlation-polarization model for molecular scattering based on free-electron-gas theory has been tested for several molecules, including H_2, N_2, and HCl. Calculations of vibrationally elastic scattering by HCN, and of vibrational excitation of HCl in the adiabatic-nuclei approximation, with an exact treatment of exchange, have been completed. Code development that will lead to complete vibrational close-coupling calculations, with exact exchange, is in progress.

New York University
New York, New York 10003

271. *Energy-Related Atomic and Molecular Structures and Scattering Studies*

B. Bederson, Dept. of Physics **$85,000**

A project to study atomic and molecular interactions with static and dynamic (laser) fields is in progress. An additional effort is under way to study interactions of electrons with highly polar molecules. This work is partly motivated by the goal of understanding the role played by long-range forces in atomic and molecular physics. We have just completed a study of the electric dipole polarizabilities of all the alkali-haldide dimers and of atomic indium. We have also obtained, for the first time, tentative values for monomer polarizabilities of several alkali-haldides. Collision experiments executed involve scattering of slow electrons (~0.5 to 20 eV) by alkali-haldide molecules and their dimers. Absolute values of effective cross sections for CsBr, CsCl, KI, RbBr and RbCl have been obtained. These can be directly compared with computations by folding the latter into our known apparatus parameters. A systematic study of similar cross sections using other molecules possessing a range of dipole moments is also in progress. Extension of the scattering measurements to dimers, trimers, and to state-selected monomers, is also under way.

Rice University
Houston, Texas 77005

272. *Theoretical Atomic and Molecular Sciences*

N.F. Lane, Dept. of Physics **$110,000**

Theoretical quantum-mechanical and semi-classical methods are used to investigate various atomic and molecular collision phenomena of fundamental interest and, in some cases, that are relevant to dense, high-temperature plasmas and other energy research environments. Current research projects include: (1) development and application of L^2 methods to Penning ionization of alkali atoms (and eventually clusters) in slow collisions with metastable helium atoms; (2) inelastic ion-ion and electron-ion scattering in dense, high-temperature fusion plasmas; (3) excitation and excitation-transfer in slow collisions between highly-excited atoms and molecules; (4) ro-vibrational excitation in electron-molecule radiative and non-radiative charge-transfer collisions; and (5) related topics.

Smithsonian Astrophysical Observatory
Cambridge, Massachusetts 02138

273. *Measurements of Ionization Balance Parameters in Atomic Ions*

J.L. Kohl, Division of Atomic and Molecular Physics **$100,000**

The purpose of this research project is to measure the basic atomic parameters that govern the charge distribution of atomic ions in high temperature plasmas. The present research efforts are directed toward measurements of absolute cross sections for dielectronic recombination of a multiply charged atomic ion and a free electron. This process is believed to dominate the ionization balance of impurity ions in potential controlled thermonuclear plasmas. The measurements utilize inclined electron and ion beams and, in the experiments, ion-photon pairs of recombined ions and stabilizing photons from individual dielectronic recombination events are measured in coincidence to ensure the correct identification of the detected process. The present activity is a measurement of the dielectronic recombination cross section for C^{3+}. Several modifications have been made to the experiment to reduce the accidental coincidence rate to an acceptable level.

SRI International
Menlo Park, California 94025

274. *Studies of Autoionizing States Relevant to Dielectronic Recombination*

T.F. Gallagher, Molecular Physics Lab. **$77,000**

The goal of this project is the study of doubly excited atomic states of alkaline earth atoms which lie above the lowest ionization limit and thus autoionize. This is of practical importance since dielectronic recombination of ions and electrons via autoionizing atomic states plays an important role in energy loss from tokamak plasmas. Both the intrinsic properties of the atoms and the effects of external fields are investigated. The approach employed is multistep laser excitation of atoms in a thermal beam, followed by subsequent detection of the ions and electrons produced by autoionization. The high resolution of the laser affords an excellent spectral probe of the autoionizing levels, and energy analysis of the ejected electrons allows the final state to be unambiguously determined. In fact, this approach is precisely the inverse of dielectronic recombination. We are thus able to probe in detail many of the phenomena associated with dielectronic recombination in plasmas.

St. John Fisher College
Rochester, New York 14618

275. ***Multilevel Relaxation Phenomena and Population Trappings***
F.T. Hioe, Dept. of Physics **$60,000**

This research program undertakes the following studies: (1) the newly discovered theory of multilevel adiabatic following will be extended to the study of selective multistep photoionization; (2) experiments will be suggested for observing multiphoton echoes and for understanding multiphoton relaxations; (3) a more complete theory of Landau-Zener effect at avoided crossings for multilevel systems will be formulated in relation to the optimum rate for accomplishing population inversion; and (4) multiple pulse propagation and the possibility of observing self-steepening or optical shocks will be explored.

Texas A & M University
College Station, Texas 77843

276. ***X-Ray Emission in Heavy-ion Collisions***
R.L. Watson, Dept. of Chemistry **$68,900**

High resolution x-ray spectral measurements are being performed for the purpose of investigating: (1) rapid electron transfer in light elements following multiple ionization by fast heavy-ion impact; (2) excitation and x-ray emission from np states of fast heavy ions in gaseous and solid media; and (3) alignment of P states in ion-atom collisions. Spectra are obtained using a variety of beams, ranging from protons to argon ions provided by the Texas A&M variable energy cyclotron. The objectives of these experiments are to obtain a basic understanding of the processes responsible for chemical effects on x-ray satellite and hypersatellite structure, and to characterize solid state influences on x-ray emission from few-electron heavy ions, including alignment and possible coherence effects.

University of Arkansas
Fayetteville, Arkansas 72701

277. ***Theoretical Study of Electron Capture in Ion-Atom Collisions***
M. Lieber, F.T. Chan, Dept. of Physics **$42,000**

Electron capture processes in ion-atom and ion-ion collisions (e.g., $A^+ + B$ yields $A + B^+$) are of importance to several areas of research, such as the controlled fusion energy program, astrophysics, and atmospheric phenomena. As a prototype of a rearrangement collision that is experimentally accessible, charge exchange has been studied since the earliest days of quantum mechanics, but the difficulty of calculation has limited theoretical progress. Recent work has shown that eikonal techniques can be successfully applied to problems of this type, and have surprising power and simplicity. Calculations are being performed on: (1) simultaneous capture of two electrons in He^{++} collisions with neutral atoms; (2) the connection between the eikonal approximation and asymptotic behavior of the wave function; and (3) the effect of Stark-mixing of energy levels on electron capture cross sections for capture into a subshell. We have recently turned our attention to multiphoton processes, which are of considerable interest both in terms of basic theory and in various practical applications. Previous theoretical work reported so far on absorption and ionization processes has involved only a single light beam. We plan to generalize the analysis of the two-photon process to the case of two incident light beams having arbitrary direction and polarization.

University of Chicago
Chicago, Illinois 60637

278. ***Basic Studies of Atomic Dynamics***
U. Fano, James Franck Institute **$75,000**

This project aims at describing and predicting the correlations and the energy transfers among the variables of atomic and molecular systems. The observed but paradoxical stability of resonant states that are localized on top of potential barriers, rather than on valley bottoms, seems to have been eventually understood. It derives from a general property of light or particle beams focused about a symmetry axis or plane. Whichever action produces the focusing also confines the associated transverse wave, causing it to acquire a discrete stable spectrum. This concept is being developed into a semianalytic description of a WKB wave function with some channel components propagating on top of the barrier and others in the valleys. The initial application will construct the theory of the quasi-Landau resonances of Rydberg spectra in a magnetic field, but it should bear on all atomic and molecular reactions. Other current research on novel aspects of electron mechanics is progressing regularly.

University of Colorado
Boulder, Colorado 80309

279. ***Spectroscopic Diagnostics of Electron-Atom Collisions***
A.C. Gallagher, Joint Institute for Laboratory Astrophysics **$78,000**

An experiment has been designed and construction has been initiated to measure cross sections for electron excitation of metal atoms. The experiment is designed to yield differential cross sections for spin changes as a function of electron scattering angle. The experimental plan utilizes laser excitation to high levels of atoms first excited by electron collision, and detection of the resulting fluorescence from a beam of atoms in a magnetic field. Each sublevel excited by the electrons is spectrally resolved and partial cross sections for exciting each state are obtained from the optical excitation spectrum. The atomic recoil energy distribution resulting from the electron excitation is obtained from the doppler shift of the absorption line from each substate.

280. *Near-Resonant Absorption By Atoms in Intense Fluctuating Fields*
S.J. Smith, Joint Institute for Laboratory Astrophysics **$56,700**

This research is directed to the measurement of photon absorption by atoms immersed in very intense laser radiation fields, near an atomic resonance. A primary objective is the accurate comparison of atomic absorption in a strong monochromatic field with the absorption in a strong field on which statistically well-characterized frequency fluctuations are superimposed. A hybrid system of electro-optic and acusto-optic modulators is used to impose laser bandwidths up to 30 MHz, and bandshapes out to 1 GHz from line center, on a single-mode laser beam. Lineshapes ranging from Gaussian to Lorentzian are synthesized by controlling the time scale of the fluctuations. The role of fluctuations in nonlinear atomic absorption is measured in the two-photon 3^2S-5^2S transition in sodium, in a Doppler-free configuration, and also in the saturated $3S_{1/2}(F=2,M_F=2) \rightarrow 3P_{3/2}(F=3,M_F=3)$ transition in a highly collimated atomic beam using an optical double resonance technique to study broadening, shifting, and splitting of the upper level as a function of laser intensity, detuning, and fluctuation parameters (linewidth and lineshape).

University of Georgia
Athens, Georgia 30605

281. *Quantum Mechanical Studies of Heavy Ion Scattering Processes*
T.G. Heil, Dept. of Physics and Astronomy **$54,000**

This research project concentrates on low to intermediate energy processes where a quantum mechanical description is most appropriate. Several heavy ion processes involving important constituent reactions that take place in terrestial and astrophysical plasmas are being studied in detail. Angular distributions are being calculated and interpreted for charge transfer reactions and other low energy heavy ion processes. These may prove to be a sensitive probe of the dynamics of low energy many-body collisions. Charge transfer processes between hydrogen atoms and multiply charged ions by both radiative and nonradiative mechanisms are also being studied. The charge transfer reactions [$C^{2+} + H \rightarrow C^+ + H^+ + h\nu$] and [$Al^{3+} + H \rightarrow Al^{2+} + H^+$] are being examined in detail.

University of Kansas
Lawrence, Kansas 66045

282. *Theoretical Studies of Many-Body Processes in Atomic and Molecular Physics*
S.-I. Chu, Dept. of Chemistry **$64,000**

The fundamental goals of this project are to develop new theoretical formalisms and practical numerical methods for probing intense field atomic and molecular multiphoton processes. Several new developments in semiclassical Floquet theory and quasienergy methods are currently under investigation: (1) extension of conventional one-mode Floquet theory to the many-mode theory, allowing exact treatment of multiphoton excitation processes in the presence of more than one laser field; (2) nonadiabatic theory for studying resonant IR multiphoton absorption spectroscopy; (3) most probable path approach for selecting the most important multiphoton excitation path, using artificial intelligence algorithms, allowing the study of multiphoton dynamics to very high order; and (4) coupled dressed-quasimolecular-states approach for the study of laser-assisted charge-transfer reactions in slow ion-atom collisions.

University of Missouri/St. Louis
St. Louis, Missouri 63121

283. *Low Energy Ion-Neutral Collisions*
J.J. Leventhal, Dept. of Physics **$70,000**

This experimental project is designed to investigate energy transfer and energy conversion in atomic and molecular interactions. Current emphasis is on the study of interactions involving atoms in specific (laser-excited) electronic states and the study of laser-induced processes of a type that could "turn on" certain chemical reactions. By using both spectral analysis of the radiation emitted by the reaction products and mass analysis of ionic products, nearly complete characterization of the interactions can be achieved. Of particular interest at this time is examination of the microscopic processes that are steps in the complicated sequences of reactions that collectively produce macroscopic effects, such as plasma formation, by coupling laser energy to gases or vapors. The possibility of modifying these macroscopic effects using laser-induced chemistry is also being investigated.

University of Nebraska
Lincoln, Nebraska 68588-0111

284. *Hyperspherical Coordinate Theory of Two-Electron Processes*
J.H. Macek, A.F. Starace, Dept. of Physics and Astronomy **$65,000**

In this project electron correlations are studied in two electron atoms using theoretical methods employing hyperspherical coordinates. The doubly differential cross section for detachment of H^- by impact with He is studied using adiabatic hyperspherical coordinate initial and final state wavefunctions to compute the H^- form factors. The detached electron's angular distribution is highly sensitive to electron correlations. A pseudo-state method is developed to correct the gross inaccuracies of adiabatic hyperspherical wavefunctions at large radial distances. This procedure yields significantly improved ^1S elastic phase shifts for electron scattering on atomic hydrogen. The Fock series expansion for two electron wavefunctions has been successfully implemented numerically. When matched to single channel adiabatic functions for some radius R_0, the Fock wavefunctions for He amd H^- differ little (for $0 < R < R_0$) from the adiabatic wavefunctions, at least for the lowest adiabatic channels. This confirms other recent theoretical results. The R-matrix for systems of coupled differential equations containing first derivative coupling matrix elements is found to be asymmetric. An alternative matrix (equal to the sum of the inverse R-matrix and the first derivative coupling matrix) is found to be symmetric. The Wannier threshold energy dependence of cross sections and angular distributions is derived quantum mechanically for the Coulomb breakup of three-particle systems with arbitrary angular momentum.

University of New Mexico
Albuquerque, New Mexico 87131

285. Atomic Physics With Relativistic Beams
H.C. Bryant, Dept. of Physics and Astronomy **$95,000**

Exploitation of the relativistic kinematics of an 800 MeV H beam at the Clinton P. Anderson Meson Physics Facility (LAMPF) at Los Alamos allows the observation, with very little background, of the one and two electron continua and embedded resonant structures. The H system is being studied using Doppler-tuned laser probes and motional electric fields, which have so far ranged up to 7 MV/cm, far in excess of those possible using more conventional laboratory techniques. The behavior of the H system as a function of both excitation energy and applied field is being carefully mapped out. Energy scale calibration is provided by excitation, with single photon absorption, of the Lyman series in an H^0 beam, derived from the H beam by photodetachment. The studies of the ^1P resonant structures in H near n=2, the shape and Feshbach resonances, and that of the 2 electron threshold region are proving to be exceptionally challenging to atomic physics theory, and more detailed measurements in these regions are planned.

University of North Carolina
Chapel Hill, North Carolina 27514

286. Experimental Studies of Atomic Inner Shell Ionization Phenomena
S.M. Shafroth, Dept. of Physics and Astronomy **$70,200**

This project is designed to study inner-shell vacancy production in ion-atom collisions, and subsequent decay via x-rays or Auger electrons. A position sensitive parallel plate electron spectrometer has been developed, and used to study metastable Auger electron emitting ion beams. A new design for high resolution projectile electron spectroscopy is in progress. Primary emphasis at this time is on experiments relating to dielectronic recombination. In a typical experiment, beams of fast, highly stripped ions, such as Si^{11+} produced by the TUNL FN tandem Van de Graaff accelerator, are directed to interact with a helium gas target. The charge state of the projectile ion is then analyzed by means of an array of four parallel plate avalanche detectors. K-shell x-rays, which are detected with a Si(Li) detector in coincidence with ions that have captured or lost one or two electrons, are recorded. The charge transfer cross sections (i.e., electron capture and loss probabilities) are also measured directly, as are prompt and metastable K x-ray yields, K vacancy sharing cross sections, and radiative electron capture (REC). Each of these quantities is then compared with theory.

University of Oklahoma
Norman, Oklahoma 73019

287. Experimental and Theoretical Study of Very Low Inelastic Processes in Electron-molecule Collisions
M.A. Morrison, Dept. of Physics and Astronomy **$27,000 (6 mo.)**

The research project involves a comprehensive theoretical and experimental study of very-low-energy electron-impact excitation of molecules. This research is directed at determining reliable cross sections for molecules of basic scientific interest and of relevance to technological applications such as advanced energy programs. The project seeks to resolve significant discrepancies that exist among the results of various experimental and theoretical investigations of near-threshold excitation of molecules by low-energy electrons, and to develop a deeper understanding of the physics of this important collision process. In the experimental part of the program absolute differential cross sections for low-energy, electron-impact excitation of these molecules shall be measured using a crossed-beam time-of-flight (TOF) apparatus which is especially suited to low-energy collision studies. The theoretical work entails carrying out accurate *ab initio* calculations of cross sections for vibrational and rotational excitation, and developing new methodologies for handling collisions with large complex molecular targets in the near-threshold energy regime.

University of Rochester
Rochester, New York 14627

288. Nonlinear Optics With Broad-Band Lasers
M.G. Raymer, Institute of Optics **$70,000**

Experiments are being carried out to understand the statistical properties of broad-band laser radiation, and the effects of using such radiation in several areas of nonlinear optics. Intensity fluctuations and mode correlations are being studied in both cw and pulsed broad-band dye lasers via intensity autocorrelation and spectral measurements. Such broad-band lasers are used to pump stimulated Raman amplification, and coherent anti-Stokes Raman scattering in hydrogen gas. Intensity and field cross-correlations which develop between pump and probe laser beams in these processes are being observed, using an intensity cross-correlator and a nonlinear interferometer based on the interference of beams produced at the sum-frequency of the two beams of interest.

University of Tennessee
Knoxville, Tennessee 37996-1200

289. Production and Destruction of Metastable Negative Ions
D.J. Pegg, Dept. of Physics **$44,400**

This research project is designed to investigate the production and destruction of metastable negative atomic ions. In particular we begin our measurements on Ca^-, where the $4s4p^2\ {}^4P$ state is theoretically predicted to be bound and metastable against allowed radiative and autodetachment decay mechanisms. Our source of negative ions is a fast moving beam, and we plan to use electron spectroscopic techniques to study the energy of electrons detached in flight by the processes of autodetachment, collisional detachment, and photodetachment.

University of Texas
Austin, Texas 78712

290. Kinetic Studies Following State Selective Laser Excitation
J.W. Keto, Dept. of Physics **$74,000**

Electronic energy transfer from xenon atoms and excimers is studied following selective excitation by multiphoton laser excitation. Reactions at higher pressures where termolecular processes are observed are being emphasized. Initial experiments are studying radiative lifetimes and quenching of $5p^5 6p$ xenon atoms in collisions with xenon and other rare gases. Accurate potential curves for xenon excimers are obtained by comparison of two-photon spectra with line broadening theories. Comparisons are made over a broad range of temperatures and pressures. Collisional deactivation rates are being measured. These rates are found to be dependent upon laser frequency. Atoms which absorb in the red wing of an absorption are excited as collision pairs at a unique inter-nuclear separation; hence, the laser prepares the reactant selectively on the collision surface. Experiments studying laser controlled reactive transfer are planned.

University of Toledo
Toledo, Ohio 43606

291. Semiempirical Studies of Atomic Structure
L.J. Curtis, Dept. of Physics & Astronomy **$55,000 (24 mo.)**

The structure and properties of very heavy and very highly ionized atoms are being studied through experimental measurements utilizing fast ion beam excitation, and through the identification and exploitation of regularities in the data base using precise empirical parametrizations. The use of spectroscopic line intensities to determine thermonuclear plasma temperatures and densities requires laboratory observation and analysis of these systems. The spectroscopic accuracies required are difficult to achieve by purely *ab initio* theoretical methods for many complex electron systems in this highly relativistic regime. Through the acquisition and systemization of experimental data, regularities and linearities are being utilized to predict a wide variety of atomic structure properties, which are subsequently tested experimentally. Recently, special emphasis has been given to the prediction of wavelengths and transition probabilities for metastable states in highly ionized atoms that decay by magnetic dipole, electric quadrupole, or spin-mixing processes, which are observed in Tokamak spectra.

Vanderbilt University
Nashville, Tennessee 37235

292. Theoretical Studies of Atomic Transitions
C. Froese Fischer, Dept. of Computer Science **$82,000**

The present research is part of an ongoing project in atomic structure calculation with special emphasis on the prediction of energy levels and transition probabilities as well as lifetimes. The method used is the MCHF method for including correlation effects in the wavefunction, optionally corrected for relativistic effects in the Breit-Pauli approximation. Transitions of current interest are the forbidden transitions which may be important in astrophysics for the electron density, or which have been observed in Tokamak plasmas. Also of interest are the transitions between the doubly excited states of Ca II, where predicted wavelengths and lifetimes are needed to identify lines of observed spectra. The present general purpose programs for the study of bound-bound transitions are being extended to include photoionization studies which may be characterized as bound-continuum transitions.

Western Michigan University
Kalamazoo, Michigan 49008

293. Correlated Charge Changing Interactions and K X-Ray Emission in Ion-Atom Collisions
E.M. Bernstein, J.A. Tanis, Dept. of Physics **$60,000**

An experimental program to probe fundamental interactions in ion-atom collisions is being conducted. Individual inner-shell processes of excitation, ionization, and charge transfer are investigated for highly charged ions (12 » Z » 26) incident on gas targets under single collision conditions. Cross sections for the various processes are measured for a range of projectile velocities (0.5 MeV/amu to about 8.0 MeV/amu) and incident charge states for several projectile and target species. Experimentally, this work is carried out by measuring coincidences between x rays (from the projectile and/or the target) and the outgoing projectile charge state of interest. Specific topics being investigated are: (1) resonant-transfer-and-excitation and associated processes; (2) excitation and ionization of projectiles and targets; and (3) electron capture to excited states (n « 2) for hydrogenlike and bare projectiles. In addition, total cross sections for electron capture and loss are obtained. These results, when taken together, provide a rather complete picture of the collision dynamics for the projectile-target combinations investigated.

Chemical Energy

Brigham Young University
Provo, Utah 84602

294. Metal Support Interactions: Their Effects On Catalytic Properties of Cobalt
C.H. Bartholomew, Dept. of Chemical Engineering **$71,800**

Metal-support interactions and their effects on adsorption and activity/selectivity properties of cobalt are being investigated. The objectives of this study are: (1) to determine the effects of cobalt-support interactions on dispersion, oxidation state, and adsorption properties of cobalt; (2) to correlate the catalytic properties for hydrocarbon synthesis on cobalt with dispersion, oxidation state, and CO and H_2 adsorption properties; and (3) to measure directly the extent of interaction of various supports with iron and cobalt using Moessbauer Spectroscopy. The work features a comprehensive, quantitative experimental investigation of Co on Al_2O_3, SiO_2, TiO_2, MgO, and carbon supports including careful characterization of the physical and chemical, bulk and surface properties of each catalyst with BET, H_2 and CO chemisorptions, XRD, TEM, TPD, and TPR measurements. Recent results provide evidence that dispersion and support significantly influence adsorption and CO hydrogenation activity/selectivity properties of cobalt.

California Institute of Technology
Pasadena, California 91125

295. Organometallic Catalysts and Analogs For CO Reduction and Carbon-Carbon Bond Cleavage Reactions

R.H. Grubbs, Dept. of Chemistry **$107,000**

The research is concerned with the activation and reduction of carbon monoxide. Group VI-B intramolecular metalloesters are synthesized from cationic transition-metal(II) carbonyl complexes, employing intramolecular nucleophiles. Spectroscopic and x-ray crystallographic evidence confirm the general structure as an ester derived from the attack of an alkoxide at a carbonyl ligand. Equilibrium studies indicate that attack by an intramolecular nucleophile may be favored over that of an intermolecular one depending on the structure linking the nucleophile to the metal center. The optimum configuration for intramolecular nucleophilic attack is being investigated. One-electron electrochemical oxidation of an arene chromium carbonyl complex results in the rapid substitution of the carbonyl ligands by added phosphines or solvent. The intermediate was identified. A family of Group IV ketene complexes has been synthesized as models for C-C coupling intermediates in CO reduction reactions. Of particular interest are binuclear complexes which show a wide range of reactivities and structures.

Colorado State University
Fort Collins, Colorado 80523

296. Chemically Modified Electrodes and Related Solution Chemistry

C.M. Elliott, Dept. of Chemistry **$70,000**

New chemically modified electrodes and related solution chemistry are under study in this research. The goal is to alter the kinetics of electrode reactions in a useful way. Of primary interest is the catalysis of various kinetically inert small molecules that are of economic interest; in particular, the respective four electron and six electron reductions of dioxygen and dinitrogen. Different synthetic procedures appropriate for each of the materials under study are being investigated in order to chemically bind the potential catalyst to the surfaces of bulk electrode materials. Our primary emphasis is the development of polymer coated electrodes containing the potential catalyst and/or other electroactive materials. Several such electrodes have been prepared and are under active investigation. A number of novel metalloporphyrin compounds have been prepared, and their catalytic activity is presently under investigation both in solution and polymer bound. The primary methods of investigation of these surfaces are electrochemical, including such techniques as chronoamperometry, cyclic voltammetry, and the rotated disk electrode technique.

297. Diosmacycloalkanes As Models For the Formation of Hydrocarbons From Surface Methylenes

J.R. Norton, Dept. of Chemistry **$52,000**
(7 mo.)

This project develops an efficient general synthesis of diosmacycloalkanes. The project will then determine the extent to which these compounds can: (1) serve as models for methylene aggregation on the surface of Fischer-Tropsch catalysts; (2) catalyze olefin metathesis; and (3) rearrange carbon skeletons. The properties of these compounds will be compared to those of their mononuclear analogs, in order to determine which (if any) steps in typical catalytic sequences require the presence of polynuclear systems. The project will also see if hydrocarbon C-H bonds can be activated by $Os(CO)_4$ or any other species generated photochemically from $Os(CO)_5$.

298. Reactions of Alkyl Palladium and Platinum Dimers: Mechanisms of Dinuclear Elimination

J.K. Stille, Dept. of Chemistry **$68,000**

Metal clusters can serve as models for metal surfaces in catalysis, and because the cluster is well defined and amenable to study by the methods and techniques available to homogeneous systems, the reactions on clusters can be studied in detail. Thus, a knowledge of the mechanisms of reactions that occur on clusters can provide a better understanding of heterogeneously catalyzed reactions, and help in developing new heterogeneous catalysts. The synthesis of dinuclear platinum, palladium, and rhodium complexes containing organic groups on adjacent bonded metals, and the reactions of these complexes, particularly the 1,2-reductive elimination, rearrangement, oligomerization, and insertion reactions are being carried out. Elucidation of the mechanism(s) of these reactions should provide a better understanding of how coupling, oligomerization, and isomerization reactions of hydrocarbons take place on metal surfaces.

Harvard University
Cambridge, Massachusetts 02138

299. Model Studies of Hydrodesulfurization and Hydrodenitrogenation On Sulfided Molybdenum Surfaces

C.M. Friend, Dept. of Chemistry **$49,900**

This program is directed toward the study of hydrodesulfurization and hydrodenitrogenation reactions on sulfided molybdenum surfaces. Model studies on well-characterized sulfided single-crystal molybdenum surfaces will be performed, both in ultra-high vacuum and at high pressures ($\geq$ 1 atm). These complementary experiments will help delineate key factors that control C-S and C-N bond activation on sulfided molybdenum surfaces. A range of experimental spectroscopic and chemical techniques will be utilized in ultra-high vacuum in order to identify and characterize reaction intermediates and model catalyst surfaces prior and subsequent to the high pressure reaction. Reaction product distributions at high pressure will be monitored by gas chromatography and/or mass spectrometry of trapped products.

Indiana University
Bloomington, Indiana 47405

300. Metal Alkoxides–Models For Metal Oxides

M.H. Chisholm, Dept. of Chemistry **$146,500**
(24 mo.)

Structural analogies between polynuclear metal alkoxides and metal oxides have been noted, with the former providing models for subunits within the extended networks of the latter. An extensive organometallic chemistry supported by alkoxy ligands is emerging. Their facile interconversion between terminal and bridging positions and between σ^2 and $(\sigma^2 + \pi^2)$ donors allows for easy uptake and release of subtrate molecules. Key reports during the 1983-1984 period are: (1) the cleavage of C-O to carbido and oxo tungsten alkoxide clusters; (2) the coupling, cocoupling, and sometimes metathesis-like reactions (M = W) between C triple bond C, C triple bond N and M triple bond M bonds in $M_2(OR)_6$ compounds; (3) unusual β-hydrogen effects in dinuclear alkyl-alkoxides of molybdenum, and (4) the isolation of Mo-Mo quadruply bonded compounds supported by alkoxide ligands. Recent developments have led to general synthesis of hydridoditungsten alkoxide anions $W_2(\mu\text{-H})(OR)_8$ which have been isolated as sodium salts.

301. Radical Chain and Rearrangement Reactions in Coal Liquefaction

J.J. Gajewsji, K.E. Gilbert, Dept. of Chemistry **$71,000**

This project focuses on providing fundamental data for the thermal reactions of aromatic compounds that may serve as a basis for understanding coal liquefaction. It has been shown that 1,3-diarylhydrocarbons and ethers decompose by free radical chain processes in the temperature range of 310 to 390°C. Some of these species will react with lower temperature free radical initiators, and the kinetics and the thermodynamics of these reactions have been studied. Hindered phenols will inhibit radical chain reactions up to 200°C. We have also found that phenyl substituted tetralins cleave to smaller molecules via a complex series of radical rearrangements and phenyl shifts. Also, *p*-isotoluene and benzo-*p*-isotoluene, putative intermediates in the concerted retro-ene decomposition of 1,3-diphenylpropane, undergo thermal reactions with second order kinetics to give non-ene dimers and polymers respectively. Finally, alkenes have been found to oligomerize in competition with reduction to alkanes in hydrogen donor solvents.

Indiana University-Purdue University at Indianapolis
Indianapolis, Indiana 46223

302. Studies of Metal-Ammonia Interactions With Aromatic Substrates

P.W. Rabideau, Dept. of Chemistry **$54,000**

Reduction and reductive alkylations, effected by electron addition in dissolving metal systems such as sodium or lithium in liquid ammonia, can provide an important method for the solubilization of coal. This research is aimed at a better understanding of the fundamental nature of this reaction, using aromatic and polynuclear aromatics as model compounds. The intermediates in these reactions are monoanions, radical anions, and dianions, and efforts to study them involve direct and indirect methods. Direct studies include proton and carbon NMR with monoanions in liquid ammonia, whereas indirect studies involve determination of protonation sites (regioselectivity), and stereochemical outcome of alkylation. The conformational analysis of the reduced products (partially unsaturated six membered rings) is also being considered experimentally with proton and carbon NMR, as well as theoretically with force field calculations.

Lehigh University
Bethlehem, Pennsylvania 18015

303. Mechanisms and Controlling Characteristics of the Catalytic Oxidation of Methane

K. Klier, G.W. Simmons, R.G. Herman, J.E. Sturm, Dept. of Chemistry **$210,000 (24 mo.)**

The objective of this project is to investigate the role of metal and oxide catalysts on the selectivity of product composition in partial and full oxidations of methane. Studies of both the gas phase free radical pathways and the surface catalyzed reactions, as well as the interplay of the two, are incorporated in this project, using modern tools of spectroscopic characterization of gas phase intermediates (EPR, optical) and of surface intermediates (Auger/ESCA/LEED/EELS). The gas phase and surface reactions occurring during partial oxidation of methane are being analyzed separately, and the project is divided into four activities: (1) trapping, detecting, and identifying of free radicals; (2) electron spectroscopy of surface intermediates, and Auger/ESCA/LEED/TPD studies of halogen-treated palladium crystal surfaces; (3) kinetic and mechanistic study of the catalyzed combustion of methane; and (4) effects of nitric oxide.

Marquette University
Milwaukee, Wisconsin 53233

304. Polymer-Based Catalysts

S.L. Regen, Dept. of Chemistry **$60,900**

This research is aimed at developing highly active and stable polymeric catalysts for use in aqueous/liquid organic two phase and aqueous/resin/liquid organic three phase reactions. Current effort is focusing on poly(ethylene glycols) and poly(ethylene glycol)-grafted copolymers as catalysts for promoting dehydrohalogenation, alkylation, and saponification processes. Preliminary results indicate that significantly improved synthetic procedures are possible based on such catalysts, which should be amenable for a variety of laboratory as well as industrial applications.

Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

305. Reduction of Carbon Monoxide

R.R. Schrock, Dept. of Chemistry **$215,000 (24 mo.)**

The objective of this research is to learn how to reduce carbon monoxide catalytically and selectively to a two-carbon product such as ethanol, ethylene glycol, ethylene, or acetaldehyde. The approach is to discover how earlier transition metal hydride complexes can take part in unique reactions not possible with the later transition metals i.e., what new principles of catalytic reduction of carbon monoxide remain to be discovered. The project involves the synthesis of new transition metal hydrido complexes and a detailed study of how they react with carbon monoxide to give a μ-hydrido μ-formyl species. Analogous reactions employing metals which are less oxophilic are being sought. At present, we are investigating some novel tungsten hydrido clusters and complexes containing linked cyclopentadienyl ligands, including a late/early transition metal combination. The late/early transition metal complex is being tested for activity under typical syngas conditions.

National Bureau of Standards
Washington, District of Columbia 20234

306. Structure and Reactivity of Chemisorbed Species and Reaction Intermediates
T.E. Madey, R.D. Kelley, Division of Surface Sciences **$126,000**

This project addresses the structure and reactivity of adsorbed molecules both on single crystal catalysts and on high area catalysts using a variety of experimental methods. It involves four areas of research which have a common theme, the investigation of surface processes related to catalytic chemistry: (1) the role of catalyst promoters and poisons (Na,S,O) in inducing new surface structures in molecular complexes adsorbed on metal and oxide surfaces is being studied, using the electron stimulated desorption ion angular distribution (ESDIAD) method; (2) vibrational spectroscopy of the adsorption, decomposition, and reaction kinetics of CO, O_2, H_2O and NH_3 on single crystal metal and oxide surfaces is being studied, using high resolution electron energy loss spectroscopy (EELS); (3) neutron inelastic scattering (NIS) is being used to characterize the vibrations of surface species on Raney Ni and Pt-black catalysts, and the utility of NIS as an *in situ* surface vibrational probe of CO hydrogenation under reaction conditions is being pursued; and (4) hydrogenation and hydrogenolysis reactions over single crystal catalysts (tungsten, tungsten carbide, Cu/Ni alloys, and small particles supported on oxide surfaces) are under investigation.

Northwestern University
Evanston, Illinois 60201

307. Solid State, Surface, and Catalytic Studies of Oxides
H.H. Kung, Dept. of Chemical Engineering **$88,600**

The purpose of this project is to elucidate the interrelation among the solid state, surface, and catalytic properties of oxides. Current emphasis is on the effect of crystalline size and surface atomic structure in surface chemistry and catalysis. In the former, Fe_2O_3 catalysts of average crystallite sizes ranging from 2.5 to over 100 nm were prepared. Moessbauer, x-ray, and magnetization measurements indicated the presence of only α-Fe_2O_3. When used as catalysts for butene oxidation, the selectivity for butadiene was found to decrease from about 80% to less than 40% with increasing crystallite size. In the study of surface atomic structure effect, single crystal planes of (0001), $(10\bar{1}0)$, $(40\bar{4}1)$, and $(50\bar{5}1)$ of ZnO were used in the decomposition of methanol, formaldehyde, and formic acid. The product distributions on $(10\bar{1}0)$, $(40\bar{4}1)$, and $(50\bar{5}1)$ were the same, but the decomposition activity increased with step density. The primary reaction is the oxidation to formate which decomposed into CO, CO_2, H_2, and H_2O. On the (0001) surface, in addition to oxidation, a dehydrogenation pathway also exists to yield formaldehyde, H_2, and CO from methanol.

308. Supported f-Element Organometallic Complexes: Surface Chemistry and Catalysis
T.J. Marks, R.L. Burwell, Jr., Dept. of Chemistry **$71,000**

This project involves a study of the surface chemistry and catalytic activity of organoactinide complexes deposited on oxide supports. Two complexes, M = Th, U in $M[(CH_3)_5C_5]_2(CH_3)_2$ had been found to give very rapid hydrogenation of propylene at -63°C, and polymerization of ethylene at 25°C. $Th[(CH_3)_5C_5]_2H_2$ dimer and $Th[(CH_3)_5C_5](benzyl)_3$ have now been found to exhibit similar or higher activity for hydrogenation, but $U[(CH_3)_5C_5]_2(CH_3)Cl$ has only 5% as much activity. Poisoning experiments with CO indicate that only a few percent of the U or Th atoms become active sites for these reactions. During activation, a fraction of $U[(CH_3)_5C_5]_2(CH_3)_2$ loses methane to form the alkylidene $U{=}CH_2$, probably stabilized by interaction with surface Al. A number of the adsorbed species have been directly observed by high resolution solid state nmr techniques.

309. Chemical Interactions in Bimetal/Zeolite Catalysts
W.M.H. Sachtler, Dept. of Chemistry **$82,600**

For zeolite supported metals, the catalytic potential of bi- or multi-metal catalysts is still basically unexplored. An essential prerequisite for the development of this field is to enhance the interaction of transition metals with the zeolite framework, in order to impede migration of metal atoms to the outer surface, where they agglomerate to large particles. The primary objective of this research is, therefore, to improve the interaction between transition metals and zeolites. The ability of ions with unfilled d- or f-orbitals of appropriate energy to act as "anchors" for reduced transition metals is investigated. The dispersion of metals (e.g., Pt or Rh on zeolites doped with Fe^{3+} or Cr^{3+}) is studied. Claims in the literature that such ions enhance the dispersion of Pt are verified. ESR or EXAFS will be used to identify the valency of the ions after reduction and the interaction of paramagnetic ions with metal atoms. The catalytic performance of the bimetal/zeolite combinations is studied, using the hydroisomerization of methyl cyclopentane as an allegedly structure-sensitive test reaction, and compared with the performance of the monometal/zeolite reference systems. While attention is mainly focused on effects due to enhanced dispersion maintenance, we also look for indications that catalyst selectivities and/or activities are affected, as found previously for bimetal catalysts on other supports.

310. Structure and Chemistry of the Interaction of Organometallics With Surfaces
D.F. Shriver, Dept. of Chemistry **$94,500**

The objective of this research is to characterize organometallics attached to surfaces. The primary techniques include quantitative analysis of gases evolved upon interaction of the organometallic with the surface, Fourier transform infrared spectroscopy, Raman spectroscopy, and extended x-ray absorption fine structure. Initial studies will center on metal carbonyls attached to the metal oxide surfaces. Parallel studies will be performed on molecular compounds which simulate the proposed surface species. Catalytic activity of some of the surface organometallics will be investigated.

Owens-Illinois, Inc.
Toledo, Ohio 43666

311. Investigation of the Nature of Semisynthetic Esterases

M.H. Keyes, Dept. of Biotechnology **$69,400**

This research project is designed to study the nature of semisynthetic esterases, generated from nonesterase proteins, by means of conformational modifications induced by inhibitors of natural esterases. Two esterases are being generated from bovine pancreatic ribonuclease, using indolepropionic acid as the modifier, after perturbing the protein under acid pH and cross-linking with glutaraldehyde. The esterase activity is assayed using tryptophan ethyl ester as substrate and measuring the ethanol produced. The two esterases are distinguished by their distinct pH optima, substrate specificity, and inhibition by tryptophan. After separation by ammonium sulfate precipitation, further purification of the esterases is being accomplished by gel filtration. The specificity of the esterases is being investigated using various esters, and amide substrates. Kinetic studies on the most appropriate substrates are being done.

Pennsylvania State University
University Park, Pennsylvania 16802

312. Mechanistic Studies of Carbon Monoxide Reduction

G.L. Geoffroy, Dept. of Chemistry **$78,600**

Mechanistic schemes for the metal surface catalyzed reduction of carbon monoxide to methanol and to hydrocarbons have been proposed, and the feasibility of these mechanisms is being tested by preparing and studying the chemistry of metal clusters which resemble the proposed surface intermediates. Initial focus was on the preparation and reactivity studies of cluster complexes bearing formyl and acyl substituent groups. The stepwise reduction of CO to CH_4 on an Os_3 cluster via a formyl intermediate was observed. More recently it has been found that $Os_3(CO)_{11}(\mu\text{-}CH_2)$, an isolatable intermediate in the preceding transformation, reacts readily with CO to yield the first ketene substituted cluster, $Os_3(CO)_{12}(\eta^2(C,C)\text{-}\mu_2\text{-}CH_2CO)$. This species has been characterized spectroscopically and by a single crystal x-ray diffraction study; its chemistry is now being explored in detail. A series of mixed-metal dinuclear complexes have been synthesized, and their CO/H_2 reactivity is being examined. Focus is on dinuclear complexes containing one early and one late transition metal and held together by bridging $\mu\text{-}PR_2$ groups.

313. The Nature of the Contribution of the Polymers of Cell Walls of the Higher Plants to Coal Formation

P.H. Given, Coal Research Section **$55,000**

The objective of this project is to identify in peats the chemically altered forms of the plant polymers that constitute the input to coalification. Cores from four sites in the Florida Everglades and Okefenokee swamp have been obtained. About 30 to 50% of the organic matter in all levels of a peat derived from the red mangrove consists mostly of tissue from the rootlets and secondary roots of the tree. Specimens of these organs hand-picked from the upper layers of the peat show strong carbohydrate character, judging from FTIR and ^{13}C nmr spectra, but are not purely cellulosic. Nevertheless, the abundant rootlets from +40 mesh sieved material has a pronounced aromatic character, which resembles but is not identical with lignin, apparently because the rootlet material is encrusted with brown amorphous (humic?) substances. It has been found that oxidation with pertri fluoroacetic acid almost completely destroys cellulose but with lignin gives a good yield of a rather small number of simple polycarboxylic acids. The method has promise for the study of peats. In summary, the peat studied contains both carbohydrate- and lignin-related substances, but these are not identical with the natural polymers.

314. Characterization of Active Sites and Their Role in Gas-carbon Reactions

R.G. Jenkins, P.L. Walker, F.J. Vastola, Dept. of Chemistry **$88,800**

This research project is concerned with measuring the concentration of active sites on carbons varying in crystallite size and orientation (all the way from microporous carbons of poor crystallinity to natural graphite flakes of high crystallinity), and relating this concentration to gasification rates. Previous work has shown that the steady state gasification rate at 0.1 MPa O_2 correlates with the total amount of surface oxide, and that CO can inhibit the steady state gasification rate. Current work is focused on characterizing the surface oxide formed during steady state gasification under varying conditions of temperature, pressure, and duration of reaction. The $C\text{-}O_2$ reaction is significantly catalyzed by Pt; e.g., the rate is about 400 times larger for 1% Pt deposited on a graphitized carbon black compared to the uncatalyzed case at 775 K and 0.1 MPa air. The reaction rates (673-773 K and 0.01 to 0.1 MPa O_2) are found to depend on the amount of Pt on the sample. The Pt dispersions on various samples are being determined by an x-ray line broadening and $O_2\text{-}CO$ titrations at 298 K. The rate constants are found to be independent of average Pt dispersions.

315. Transition Metal Catalyzed Transformations of Unsaturated Molecules

A. Sen, Dept. of Chemistry **$71,000**

The present research is concerned with the study of several novel homogeneous transition metal catalyzed reactions. A common feature of these catalytic processes is the use of relatively inexpensive small molecules (e.g., olefins and carbon monoxide) as building blocks in catalytic cycles to make more elaborate, larger molecules. The catalytic reactions currently under study are: (1) the stereospecific tail-to-tail dimerization of alkyl acrylates; and (2) the copolymerization and cooligomerization of carbon monoxide with olefins, dienes, and acetylenes. The latter transformations, under mild conditions, were discovered by us in the course of our previous studies. Since these catalytic processes are of considerable interest from a practical standpoint, we have undertaken a detailed study of their mechanism and scope. We expect to use the insight gained from such a study to tailor catalysts for higher specificity and/or milder reaction conditions.

316. Metal-Support Interactions in Ni, Pd, and Pt Catalysts

M.A. Vannice, Dept. of Chemical Engineering **$81,500**

This research project is directed toward a better understanding of the chemistry involved in the creation of metal-support interactions in certain systems, which have been found to have pronounced effects on adsorption and catalytic behavior. This project involves a study of heats of adsorption and adsorption/desorption behavior for H_2, CO and O_2 on Pt, Pd, and Ni, using a modified differential scanning calorimeter and a thermal gravimetric analysis unit. Kinetic investigations are being made on the hydrogenation of carbon monoxide and aromatic hydrocarbons, beginning with benzene. Possible correlations between catalytic activity and adsorbate-metal bond strengths are being investigated. Recent results indicate that activity enhancement is due to additional active sites occurring in the metal-support interface region, and that surface bond strengths do not decrease on TiO_2-supported Pt and Pd although adsorption decreases markedly. This multifaceted approach should provide a more complete explanation of both the much higher catalytic activities already found in certain reactions and the suppressed chemisorption which is observed after the SMSI state is induced.

Purdue University
West Lafayette, Indiana 47907

317. *Reduction of Aromatic Compounds Derived From Coal By Calcium*
R.A. Benkeser, Dept. of Chemistry **$60,000**

The versatility of the new reducing system consisting of calcium metal dissolved in a mixture of methylamine-ethylenediamine has been broadened considerably. By the simple expediency of adding an alcohol to the usual calcium-mixed amine system, it is now possible to reduce aromatic hydrocarbons which are abundant in coal to dihydro compounds (Birch-type products) rather than to tetrahydro products. Thus o-xylene can be reduced in high yield to 1,2-dimethyl-1,4-cyclohexadiene, m-xylene to 1,5-dimethyl-1,4-cyclohexadiene and p-xylene to 1,4-dimethyl-1,4-cyclohexadiene. The role played by the methylamine in these reductions is multifold. Its presence ensures that the calcium does not become coated with an insoluble substance during the course of the reduction. This coating often causes the reduction to stop and low yields of products result. This coating seems to be some type of a calcium amide. In many cases, the methylamine can be omitted and the reduction made to proceed very well in pure ethylenediamine provided a large excess of calcium is used. Another alternative which obviates the need for methylamine is to use a Hershberg stirrer and sand. The latter combination provides an abrasive action which prevents the calcium from becoming coated.

Rensselaer Polytechnic Institute
Troy, New York 12181

318. *Homogeneous Carbon Monoxide Fixation*
A.R. Cutler, Dept. of Chemistry **$185,000**
(24 mo.)

Organometallic complexes containing C_1 alkoxycarbonyl and C_2 carboalkoxymethyl ligands derived from terminally bound CO are being synthesized in order to delineate those coordinate ligand reactions and their intermediates that are viable for CO hydrogenation. The metalloester $FpCO_2CH_3$, derived from $FpCO^+$ or from Fp_2Mg/CO_2, serves as the common template in converting either CO or CO_2 into the C_1 alkyl ligand on $FpCH_2OCH_3$; Fp - (H-C_5H_5)Fe$(CO)_2$. The activated ester $FpC(OCH_3)_2^+$ thus adds hydride and gives its stable formylacetal $FpCH_2(OCH_3)_2$, which subsequently affords the desired $FpCH_2OCH_3$. The metylidene salt $FpCH_2^+$ (generated from $FpCH_2OCH_3$) picks up exogeneous CO, ascertained by a ^{13}C labeling study, and gives the stable (H^2-C,C) ketene complex $Fp(CH_2CO)^+PF_6^-$; this complex abstracts methoxide from methanol (or even $FpCH_2OMe$) and provides the carbomethoxy methyl $FpCH_2CO_2CH_3$. This ketene complex, which effectively derives from two carbonyls, therefore serves as an efficient source of a C_2 alkyl ligand that is important in CO fixation studies.

SRI International
Menlo Park, California 94025

319. *High Temperature Chemistry of Complex Vaporization/Decomposition Processes*
D.L. Hildenbrand, R.D. Brittain, **$60,900**
K.H. Lau, Physical Sciences Division

The objective of this program is to obtain fundamental thermodynamic data for a variety of high temperature vaporization/decomposition processes that are relevant to current and emerging energy technologies such as stack gas cleanup, coal gasification, hydrogen generation, and MHD. These processes are being studied by high temperature mass spectrometry, and by the torsion-effusion method so that both vapor composition and absolute pressures are determined. For substances that simultaneously undergo both decomposition and direct vaporization, particular emphasis is on quantitative determination of the relative contributions from each process, and on thermochemical characterization of the complex vapor species. Current studies are concerned primarily with metal sulfate and carbonate processes, with recent work on the sulfates of Cs, Rb, and Li, and carbonates of K and Cs. The effects of certain additives that catalyze sulfate decomposition are also being studied, since kinetic and mechanistic features have a crucial bearing on the interpretation of the dynamic effusion measurements, as well as on the technological applications of these processes.

320. *Adsorption Thermodynamics and Surface Transport of Metal Catalysts Poisons*
H. Wise, Materials Research Lab. **$76,500**

This research has for its objective a fundamental understanding of the binding energy of sulfur and halogen adatoms to metal surfaces in order to relate catalysts poisoning and reactivation to covalent bond formation. The experimental measurements involve studies of equilibrium adsorption and surface diffusion on single crystals of different orientations, and on highly dispersed metal catalysts. The techniques employed include classical studies of reversible adsorption at low surface coverages, temperature programmed desorption and surface reaction, Auger electron spectroscopy for diffusional transport, low energy electron diffraction for determination of surface coordination and reconstruction, and segregation experiments for study of the interaction of different CO-adsorbed surface species. At low surface coverage of sulfur significant variations in binding energy have been observed for different metals. Relative to Ni the sulfur adatoms are less strongly bound in the series Ni>Co>Ru>Fe>Ir>Cu>Pt. Typically the bonding of sulfur appears to involve the sp and d bands of the metals and the sulfur 3p orbitals, as observed by photoelectron spectroscopy. Theoretical correlations are in progress to relate the binding energy of sulfur to the electronic structure of the metal.

Stanford University
Stanford, California 94305

321. Catalyzed Gasification of Carbon
M. Boudart, Dept. of Chemical Engineering **$75,000**

Unsupported molybdenum carbide powders with high specific surface area and alumina supported highly dispersed molybdenum carbide clusters possess very high catalytic activity for the hydrogenolysis of n-butane. The surface of the powders normally contains polymeric carbon which must be removed by temperature programmed reduction with dihydrogen. These materials are currently investigated as new catalysts for CO-H_2 reactions.

322. Molecular Beam Studies of the Dynamics of Activated Adsorption of N_2 On W(110)
R.J. Madix, Dept. of Chemical Engineering **$218,500 (24 mo. FY 83)**

The activated adsorption of N_2 on W(110) was studied using molecular beams to achieve translational energies from 2 to 30 kcal/mol. The beams were formed in nozzles with and without helium seeding. For the lowest kinetic energy, the probability of dissociation upon collision was about 10^{-3}, increasing to 2 x 10^{-1} at energies above 20 kcal/mol. The dependence of the dissociation probability on nitrogen coverage suggested the process was direct in nature, not trapping dominated. The results show that adsorption is translationally activated, and that the reactive collision is not adequately described by a one-dimensional barrier. As the beam energy was increased, the apparent saturation coverage by nitrogen increased, producing an unusual desorption state above a nitrogen atom coverage of 2.5. Nitrogen desorbed autocatalytically from this state in a fashion observed previously for high concentrations of oxygen from Pt(100). The emergence of this state at higher surface coverages indicates that the state of nitrogen adsorbed on tungsten and other metals may be different from the state normally observed in low pressure studies. Additional measurements of the angular distribution of scattered dinitrogen indicated that the unreacted N_2 did not probe the potential energy surface for reaction. Angular profiles were observed which would be expected for quasi-elastic scattering. Similar experiments are in progress for CO_2 on Ni(100).

Syracuse University
Syracuse, New York 13201

323. Metal-Support Interactions: The Effect of Catalyst Preparation On Catalytic Activity
J.A. Schwarz, Dept. of Chemical Engineering & Material Sciences **$73,500**

That the catalytic properties of a dispersed metal are influenced by the composition of the support material and by subsequent reduction procedure is well known. Recent study suggests that the procedure by which a catalyst is prepared also influences its properties, but relatively little fundamental research on the phenomena has been reported in the literature. It is proposed that this project develop a scientific basis for design and control of catalyst systems by examining the relationship between catalyst preparation procedures and the activity, selectivity, and stability of the finished catalyst. Nickel dispersed on a series of silica-alumina supports has been chosen as the prototype system because the amount and chemical properties of the nickel can be regulated by controlling the pH of the impregnating solution. The physicochemical properties of the prepared catalysts are determined by means of temperature programmed reduction, desorption, and reaction in conjunction with gravimetric and magnetization measurements.

Texas A & M University
College Station, Texas 77843-3255

324. Catalysts and Mechanisms in Synthesis Reactions
J.H. Lunsford, Dept. of Chemistry **$80,900**

A major part of this research project is devoted to understanding the structural and electronic factors which determine the catalytic properties of supported metals, such as palladium, for the formation of alcohols. Controlled modifications of the support, for example by the addition of lithium ions, can transform an inactive catalyst into one which rivals commercial catalysts for methanol synthesis activity. Infrared experiments, using CO as a probe molecule, are under way to determine the relative amounts of Pd(111) and Pd(100) planes which are exposed on the supported catalysts. Another aspect of the research involves a study of matrix-isolated gas phase radicals, which are produced on surfaces of catalytic importance. Recent work on magnesium oxide shows that surface defects which give rise to O^- ions (V-type centers) are active for the generation of methyl radicals from methane. These centers are present only on oxygen-rich surfaces, which is surprising since magnesium oxide is normally considered to be a nonreducible oxide.

325. Catalytic Behaviors of Multi-valent Lanthanide Oxides
M.P. Rosynek, Dept. of Chemistry **$131,200 (24 mo. FY83)**

This research project involves a systematic investigation of the influence exerted by selected lanthanide oxide supports, principally those of La, Ce, Pr, and Eu on the catalytic behaviors of both well-dispersed (Pt, Rh) and poorly-dispersed (Fe, Co, Ni) transition metals, with a view toward identifying evidence for significant metal-support interactions. Supports being studied as a basis of comparison include silica, alumina, and titania. Catalytic behaviors of the various metals are being evaluated for appropriate diagnostic reactions (CO hydrogenation and paraffin hydrogenolysis/dehydrocyclization) as a function of conditions and support identity. These results are being correlated with those of accompanying characterization studies, involving infrared and x-ray photoelectron spectroscopies, transmission electron microscopy, and selective chemisorption measurements in an attempt to elucidate the nature and extent of metal-support interaction effects.

University of California/Irvine
Irvine, California 92717

326. Synthesis, Chemistry, and Catalytic Activity of Lanthanide Metals in Unusual Oxidation States and Coordination Environments

W.J. Evans, Dept. of Chemistry **$73,000**

The objective of this research project is to identify the special chemical properties of the lanthanide metals (14 heavy metals which are mined in California) and to exploit this unique chemistry to develop: (1) new materials of potential practical importance; (2) more efficient and more selective catalytic systems; and (3) new stoichiometric and catalytic reactions not presently possible with conventional catalysts. Our study of the chemistry of the lanthanide-carbon bond has led to the first molecules containing lanthanide-hydrogen bonds. These lanthanide hydrides catalytically activate molecular hydrogen, and we are studying the intermediates in this reaction to understand how to modify this reactivity in unusual ways. The reactions of the hydrides with nitriles, isocyanides, alkynes, and alkenes provide new, structurally unusual complexes whose chemistry is being examined. We are investigating the subtle factors which have major effects on the rates of several of the above classes of four-center reactions. We have developed an efficient conversion of bimetallic hydrides to structurally unique trimetallic tetrahydrides and mixed metal intermetallic tetrahydrides, which may be of interest with respect to hydrogen storage. We are studying the extension of this synthesis to larger polymetallic lanthanide polyhydrides.

University of California/Los Angeles
Los Angeles, California 90024

327. *Metallacarboranes Structurally Engineered For the Reduction of Carbon Monoxide*

M.F. Hawthorne, Dept. of Chemistry **$73,500**

This research program has been designed to develop and evaluate various metallacarboranes as homogeneous catalysts for the transformation of CO into useful chemical feedstocks. Emphasis has been placed on several areas of interest: (1) the evaluation of the activity of rhoda- and ruthenacarborane complexes as catalyst precursors for the water gas shift reaction; (2) the synthesis of heterobimetallic metallacarboranes which possess both early and late transition metal vertices for the study of metal-metal cooperativity in the reduction of CO; and (3) the preparation and screening of a series of rhodacarborane complexes as hydroformylation catalysts. The ability to synthetically engineer the structural and electronic properties of metallacarboranes has proven to be an indispensible tool. The catalyst precursors used in these studies have been shown to exhibit several novel structural features which include a structurally sensitive *closo/exo nido* tautomerism, a key feature in the ability of these species to activate small molecules such as dihydrogen.

University of California/Santa Barbara
Santa Barbara, California 93106

328. *Homogeneous Catalysis of the Water Gas Shift Reaction*

P.C. Ford, Dept. of Chemistry **$71,000**

Research is directed (1) toward elucidating fundamental mechanisms key to catalytic cycles including the water gas shift reaction, and (2) toward developing new homogeneous catalysts for such reactions. Studies in progress include kinetic investigations of important steps such as the nucleophilic activation of carbon monoxide coordinated to metal centers by a variety of species including the oxy anions HO^- and CH_3O^- ($M\text{-}CO + RO^- \rightarrow M\text{-}CO_2R^-$), the decarboxylation of hydroxy carbonyl adducts ($M\text{-}CO_2H^- \rightarrow M\text{-}H^- + CO_2$), the reductive elimination of H_2 from metal hydrides ($M\text{-}H^- + H_2O \rightarrow H_2 + M + OH$), and the substitution reactions of metal carbonyl complexes. Systems under investigation are largely drawn from those shown to have potential as homogeneous catalysts in the reactions of carbon monoxide. The elucidation of these mechanisms will provide guidelines for the molecular engineering of new and better catalysts for the production of fuels and other organic products from CO and other small molecule substrates.

329. *Reactions of Iron Atoms With Molecules in Low Temperature Matrices*

R.G. Pearson, P.H. Barrett, Dept. of Chemistry **$65,100**

The goal of this project is to study the reactivity of metal atoms and small clusters, with molecules in low temperature matrices. Moessbauer and infrared spectroscopies are used to identify the reaction products. Reactions between Fe, Fe_2, and iron clusters, and low temperature matrix isolated molecules of N_2, NO, SO_2, CH_2N_2, and other small molecules are under investigation. This investigation includes the search for bond cleaving reactions of HX and CH_3X molecules, and the study of CH_2, NH and O bound to iron atoms.

University of Chicago
Chicago, Illinois 60637

330. *Reactions of Electrophilic Reagents With Bituminous Coals: The Chemistry of the Reaction Products*

L.M. Stock, James Franck Institute **$82,600**

During the initial months of the project we have concentrated on the ruthenium(VIII) catalyzed oxidation of coal. The aromatic molecules are selectively oxidized in this process to yield simpler structures. The products derived from 20 representative molecules have been worked out and the products from a representative bituminous coal have been studied by mass spectrometry. In addition, a quantitative method based upon isotopic dilution techniques has been worked out and applied successfully for the determination of the methyl groups in coal. This information can be used to predict the quantity of methane expected during low severity pyrolyses. The electrophilic reactions of bituminous coals with mercury(II) and lead(IV) are under investigation. The plumbylation reaction of Illinois No. 6 coal yields a product which undergoes oxidative solvolysis to yield a material selectively enriched in aryl hydroxyl groups. This altered coal undergoes donor solvent liquefaction in tetralin to yield products that are more soluble in hexane than the natural material. This work should provide a more secure basis for the discussion of the role of hydroxyl groups on coal conversion and hence enable their greater control.

University of Colorado
Boulder, Colorado 80309

331. *Studies of New Elimination Reactions of Metal Complexes*

M.R. Dubois, Dept. of Chemistry **$55,600**

This project is investigating elimination and rearrangement reactions of alkyl substituents on μ_2-sulfido ligands in dimers of the general types $[CpMoSSR]_2^n$ and $[CpMo(SR)_2]_2^n$ ($n = 0, -1, -2$). It has been proposed that the sulfido ligands and metal ions may participate in these reactions to provide low-energy pathways for new reaction types. Altering the nature and charge of the bridging ligands in these complexes results in significant shifts in the observed reduction potentials. The reactivity of the sulfido ligands can be tuned in this way to interact with a range of electrophiles and nucleophiles. For example, $[(CpMo)_2S_2CH_2(\mu SCH_3)\mu S]^-$ reacts with alkynes to form dimers with alkenyl thiolate ligands. This reaction may serve as a model for a pathway for alkyne reduction involving sulfur sites in metal sulfide catalysts. New dimeric complexes of vanadium, tungsten, rhenium, and iron with bridging sulfido ligands have also been synthesized and characterized. The sulfur ligands in some of the tungsten complexes appear to react readily with hydrogen despite the fact that they are in a different electronic and structural environment than the reactive ligands in the molybdenum systems. Vanadium dimers which are isostructural with the molybdenum complexes show no evidence for ligand reactivity.

332. Promoter Modifications of Catalytic Activity and Selectivity

J.L. Falconer, Dept. of Chemical Engineering **$79,300**

The effect of alkali promoters on the activity and selectivity for CO hydrogenation is being studied on supported metal catalysts. Temperature-programmed desorption and reaction (TPD, TPR), steady-state reaction and x-ray photoelectron spectroscopy are being used. The support is shown to have a strong influence on the changes induced by the alkali promoter. On Ni/SiO_2 and Ni/TiO_2 large decreases in activity are seen; on Ni/Al_2O_3 the activity does not change significantly, and on Ni/SiO_2-Al_2O_3 the activity increases. The strong effect of the support was attributed to an interaction of the support with the promoter. Rate changes measured by temperature-programmed reaction and by steady-state kinetics are in good agreement. The decreased rates are attributed to decreased hydrogenation rates of carbon monoxide and of carbon, due to weakened hydrogen bonding. This results in large increases in olefin selectivity. The activity on Ni/SiO_2 decreased rapidly with potassium concentration. Preparation method and alkali salt used were shown to have little effect on the change in activity. On unpromoted Ni/Al_2O_3 the presence of multiple reaction sites was observed and a model was developed for the reaction.

University of Connecticut
Storrs, Connecticut 06268

333. Highly Dispersed Metal Atoms in Zeolites

S.L. Suib, Dept. of Chemistry **$50,900**

The purpose of this program is to understand ways of producing small particles of highly reduced metals in zeolites. Current emphasis is on the effect of microwave discharge methods for the synthesis of highly dispersed metal atoms in zeolite pores. The metals that we are working with are Fe, Co, and Ni. The microwave discharge procedure provides a general method to produce small metal particles on other supports such as SiO_2, Al_2O_3, polymers, and TiO_2. Characterization of these materials involves Moessbauer spectroscopy, ferromagnetic resonance, x-ray powder diffraction, and surface analyses with Auger, x-ray photoelectron spectroscopy, ion scattering spectroscopy, and secondary ion mass spectroscopy. Superparamagnetic iron (0) and cobalt (0) clusters less than 20 Angstrom in size are prepared. Another aspect of this research involves use of these zeolites in Fischer-Tropsch and methanation reactions.

University of Delaware
Newark, Delaware 19716

334. A Surface Science Investigation of Potential Intermediates, Catalysts, and Promoters in the Synthesis of Higher Alcohols By Metals

M.A. Barteau, Center for Catalytic Science and Technology, Dept. of Chemical Engr. **$72,900**

The goal of this project is to provide the fundamental knowledge required to extend recent advances in methanol synthesis catalysis to the development of selective noble metal catalysts for the synthesis of higher alcohols. The hypothesis is that surface alkoxide species are pivotal intermediates in the synthesis of higher alcohols. This study will examine the formation, stability, and reactivity of these intermediates on clean and modified surfaces of rhodium and palladium, in order to determine the properties of these metals that lead one (Rh) to be active for synthesis of higher alcohols. By studying the influence of inorganic surface promoters upon alkoxide reactivity, we will determine the ability of promoters to alter the intrinsic catalytic properties of these metals, and probe the importance of promoter electronegativity in the modification of surface reactivity. Various C_1-C_4 alcohols will be used as probe molecules in order to determine (1) the effect of hydrocarbon chain length on alkoxide stability and reactivity, and (2) the influence of interactions between the surface and the alkoxide hydrocarbon chain upon alkoxide stability. In order to study the reactions of these molecules, including the identity and kinetics of formation of both gaseous products and surface intermediates, we will apply a battery of essential surface spectroscopic techniques, including TPD, HREELS, UPS, and XPS.

University of Minnesota
Minneapolis, Minnesota 55455

335. Photochemical Properties of Transition Metal-Arene Complexes

K.R. Mann, Dept. of Chemistry **$133,900**
(24 mo.)

The photochemical reactivity of transition metal arene complexes will be studied by examining the mechanisms of the arene replacement reactions by NMR, laser flash photolysis, and classical mechanistic techniques. The intermediate species generated in these reactions will be utilized as catalytic photoassistance agents, and in the synthesis of novel organometallic complexes.

University of Nebraska
Lincoln, Nebraska 68588-0304

336. *Studies On Unusually Reactive Metal Powders–Preparation of New Organic Compounds*

R.D. Rieke, Dept. of Chemistry **$63,300**

This research project is involved with the preparation and study of highly reactive metal powders prepared by the reduction of metal salts with alkali metals. Current studies are concentrating on nickel, cadmium, uranium, palladium, and platinum. The nickel powders have been found to react rapidly with benzylic halides, and the resulting organonickel complexes yield dibenzyl. Aryl halides react rapidly with the nickel powders to produce biaryl compounds in high yields. Benzylic halides react with the nickel powders in the presence of acylhalides to produce benzyl ketones in high yields. Reactions of ROCOCOCl and benzylic halides with nickel powders yield benzyl ketones. These reactions proceed with a wide variety of substituents on the phenyl ring of the benzylic halides. Highly reactive uranium has been prepared, and found to react with a variety of oxygen containing substrates, such as nitrobenzene to yield azo benzene. The chemistry of cadmium, platinum, and palladium is also under investigation.

University of North Carolina
Chapel Hill, North Carolina 27514

337. *The Heats of Formation of Gas Phase Organo-Sulfur Molecules and Applications of ^{17}O and ^{33}S NMR to Structure Determinations*

T. Baer, S.A. Evans, Jr., Dept. of Chemistry **$70,200**

This program emphasizes photoionization and heteronuclear NMR techniques directed toward the determination of structures and energetics of organosulfur molecules. The ΔH_f° of the series: RS ⊙ [R = CH_3, CH_3CH_2,$(CH_3)_2CH$, and $(CH_3)_3C$] are being measured. In addition, the ΔH_f° of various sulfonyl compounds are being determined by bomb calorimetry to make these substances amenable for photoionization studies. Chemical oxidation of sulfenyl sulfur (-S-) to sulfones (-SO_2-) and particularly, to sulfonic acids (-SO_3H) serves to "quench" the quadrupolar broadening effect. This allows for the development of an analytical NMR technique for the rapid and accurate analysis of sulfur in organosulfur constituents in coal and petroleum extracts. Polar substituent effects on ^{33}S chemical shifts in aryl sulfones and sulfonic acids are being evaluated, as well as the possible use of magic-angle spinning techniques for determination of ^{33}S shift parameters in the solid state.

University of Pittsburgh
Pittsburgh, Pennsylvania 15261

338. *Carbidic Ad-layer As Rate Controlling Factor in CO/H_2 Catalysis*

P. Biloen, Dept. of Chemical and Petroleum Engineering **$154,000 (24 mo. 1983 Funds)**

The objective of this project is to assess the reactivity and abundance of reaction intermediates present at the surface of CO/H_2 converting catalysts during steady-state catalysis. The central question which is being addressed is to what extent carbonaceous side products control the abundancy of reaction intermediates. In a typical experiment, the isotopic constitution of the feed is being changed abruptly (e.g., $^{12}CO/H_2 \rightarrow ^{13}CO/H_2$). This leads to a transient phenomenon: the displacement of ^{12}C by ^{13}C, first in the catalyst ad-layer and then in the product. The rates of displacement contain transient-kinetic information regarding the abundancy and reactivity (i.e., lifetime) of reaction intermediates. With ^{12}CO and ^{13}CO exhibiting essentially identical reactivity, the steady-state of the system is essentially not affected by the isotopic switch. In the present setup, the rate of isotopic substitution in product is being monitored by on-line mass spectrometry. Under construction is a setup to combine this with an *in situ* IR monitored rate of isotopic substitution in the reactive ad-layer.

339. *Studies of Supported Metal Catalysts*

D.M. Hercules, Dept. of Chemistry **$85,900**

We have advanced the adaptation of spectroscopic techniques for studying catalytic surfaces demonstrating the utility of ESCA, ISS, and LRS. LRS gives structural information about bulk phases, whereas ESCA gives information about dispersed phases. We have demonstrated a correlation between ESCA, EXAFS, and PAS measurements, giving information about site symmetry of transition metals on catalysts. We have shown a correlation between reducibility of catalytic species measured by ESCA and the same quantity measured classically. We have characterized Ni species an Al_2O_3 and SiO_2 when the preparation method and Ni content of the catalysts are varied. We have determined the nature of Ni species on TiO_2, ZrO_2, and ThO_2 surfaces and their reducibility. We have studied the nature of Co species on Al_2O_3, and how they are affected by Mo or Zn, or by sulfiding. We have determined how Mo species on supported catalysts are affected by reducing or sulfiding, by the presence of Co, Ni, Zn, or by the nature of the support (Al_2O_3, TiO_2). We have studied the effect of Mo impregnation pH on the nature and dispersion of Mo species, and the catalyst hydrodesulfurization activity. For tungsten on alumina, the catalyst W species differ from Mo for the same support; W species on alumina are affected by reducing, sulfiding, or by the presence of Ni.

340. *Infrared Studies of Influence of Alkali Metals On C-O Bond in Chemisorbed Carbon Monoxide*

J.T. Yates, Dept. of Chemistry **$136,100**

This research project is designed to probe the interaction of adsorbed alkali metals with adsorbed carbon monoxide on transition metal single crystal surfaces. Information obtained by reflection IR spectroscopy, x-ray, photoelectron spectroscopy, and temperature programmed desorption will yield models of the interaction, and deeper understanding of the alkali promotion effects observed in catalytic chemistry on transition metals.

University of Rochester
Rochester, New York 14627

341. *Transition Metal Activation and Functionalization of Carbon-Hydrogen Bonds*

W.D. Jones, Dept. of Chemistry **$65,900**

This research is directed toward the activation and cleavage of carbon-hydrogen bonds by homogeneous transition metal compounds. The possibilities for forming hydridometal-aryl and -alkyl complexes and trapping these intermediates with isocyanides, olefins or acetylenes is under investigation. A reaction sequence involving trapping, insertion, and reductive elimination would yield imine or styrene products. These systems have the added feature that they can be catalytic, as the metal complexes are not consumed and the overall thermodynamics are favorable. The complexes $CpRe(PPh_3)_2H_2$ and $Fe(PMe_3)_2(CNR)_3$ both show behavior with arenes that is consistent with the functionalization scheme. The former complex catalyzes the insertion of ethylene into the C-H bond of benzene, producing ethylbenzene; the latter complex stoichiometrically converts benzene to aldimine. Other studies in progress involve the mechanism and thermodynamics of intra- and intermolecular alkane and arene C-H bond activation in the series of complexes $(C_5Me_5)Rh(PMe_2R)(R')(H)$. For R = Me there is little kinetic selectivity for the activation of arenes versus alkanes. although there is a large thermodynamic selectivity favoring arene activation. Current work with R = benzyl indicates that there is little kinetic selectivity for intramolecular cyclometallation versus intermolecular activation of neat benzene solvent, but that the cyclometallated species is favored thermodynamically.

University of Texas
Austin, Texas 78712

342. Study of Synthesis Gas Conversion Over Metal Oxides

J.G. Ekerdt, Dept. of Chemical Engineering **$53,400**

The goals of this program are (1) identification of the reaction intermediates present during CO hydrogenation reactions, (2) determination of the reaction pathways whereby the intermediates are converted into products, and (3) the development of an understanding of the causes for catalytic activity and selectivity. Direct CO hydrogenation into branched alkanes, isosynthesis, is being investigated over zirconium dioxide. High pressure (35 atm) rate studies are performed to examine the primary products and establish the kinetics of C_1 to C_4 isosynthesis product formation. Atmospheric studies are performed to determine the catalytic reactions between CO, CO_2, H_2, and the zirconium dioxide surface and to gain insight into the reactions which initiate isosynthesis. The results from both pressure regimes will be used to propose a mechanism for isosynthesis. The mechanism will be used as the basis for designing experiments directed toward the causes for metal oxide activity and selectivity.

University of Utah
Salt Lake City, Utah 84112

343. Ligand Intermediates in Metal Catalyzed CO Reduction

J.A. Gladysz, Dept. of Chemistry **$91,800**

This research program has as its basic goal the synthesis and study of homogeneous complexes containing ligand types (e.g., -CHO, =CHOH, -CH$_2$OH, C, CH, =CH$_2$, $H_2C{=}O$, -OCHO, and so forth) believed to be intermediate in the metal catalyzed conversion of CO/H_2 gas mixtures to organic molecules. Mechanistic understanding of the steps involved in catalytic CO reduction, and insight needed for the design of new catalysts, is sought. Current studies are making extensive use of optically active substrates derived from easily resolved $[(H\text{-}C_5H_5)Re\text{-}(NO)(PPh_3)(CO)]^+BF_4^-$. For instance, methylidene $(+)\text{-}(S)\text{-}[(H\text{-}C_5H_5)Re(NO)(PPh_3)(=CH_2)]^+PF_6^-((+)\text{-}(S)\text{-}1)$ couples to ethylene complex $(+)\text{-}(R)\text{-}[(H\text{-}C_5H_5)Re(NO)(PPh_3)(H_2C{=}CH_2)]^+PF_6^-$ with retention. This coupling also exhibits a remarkable degree of enantiomer self-recognition: the (+)-(S)-1 couples virtually exclusively with (+)-(S)-1, and (-)-(R)-1 couples virtually exclusively with (-)-(R)-1. The formate $(+)\text{-}(R)\text{-}(H\text{-}C_5H_5)Re(NO)(PPh_3)(OCHO)$ decarboxylates at 70-130°C to hydride $(+)\text{-}(S)\text{-}(H\text{-}C_5H_5)Re(NO)(PPh_3)(H)$ with retention. An isolable manganese α-hydroxyalkyl complex has recently been observed to undergo carbonylation to a α-hydroxyacyl complex.

344. Liquid and Solid Carbon-13 Magnetic Resonance Study of Hydrocarbons and Related Substances

D.M. Grant, R.J. Pugmire, Dept. of Chemistry **$95,000**

Work continues to focus on both liquid and solid state NMR methods applied to the characterization of carbonaceous compounds and materials important in the energy industry. Model organic compounds provide substance upon which the methods may be calibrated and standardized. Hydroaromatics, coal macerals, various fossil fuels and their precursors provide the main focus of this work. Exploratory research on single crystals has been initiated in an attempt to better understand the important dipolar dephasing experiment which is being used extensively on powders such as coals, and so forth. The dipolar dephasing rate depends on the orientation of the carbon-hydrogen bonds and basic single crystal work on hydrocarbons will provide definitive information required to get good intensity data on solid state powders. The development of an ultrahigh speed rotor is well under way. By decreasing the outer diameter, it has been possible to increase the rotation rates to 8 KHz. Reduced rotor diameters will also allow for increasing radio frequency fields at reduced power dissipation. Both effects should enhance our ability to obtain chemical-shift/J-coupled two dimensional spectra in solids.

345. Comprehensive Characterization Studies of Sulfided Molybdena Catalysts

F.E. Massoth, Dept. of Fuels Engineering **$75,500**

The goal of the present work is to characterize a wide variety of supported molybdena sulfide catalysts with a number of different characterization techniques, and determine their catalytic activities for model compounds representative of several functionalities present on these catalysts in order to relate catalytic activities to catalyst properties (viz., structure, dispersion, active sites) of the active phase. Several newer techniques not available or not employed in earlier studies, as well as some conventional ones, will be used to characterize the catalysts. These include chemisorption of selected gases, 'active OH' content of the supports, H_2S^{35} exchange, ESCA, XRD, and 'SH' content. The catalytic activities of the catalysts will be measured for HDS, HDN, hydrogenation, and hydrocracking employing model compounds representative of these catalytic functions. This program should provide insight into the major factors responsible for catalytic activity of the various functions present in these complex catalysts.

University of Wisconsin
Madison, Wisconsin 53706

346. *Mechanistic Studies Related to the Metal Catalyzed Hydrogenation of Carbon Monoxide to Hydrocarbons*

C.P. Casey, Dept. of Chemistry **$103,000**

The synthesis of organometallic compounds which contain functional groups similar to those proposed in homogeneous and heterogeneous catalyzed carbon monoxide reduction is being carried out, so that the properties and reactions of these species can be studied. This basic information should contribute to the understanding and eventual design of catalysts for the reduction of carbon monoxide. Detailed studies of the synthesis and reactions of metal formyl compounds (M-CO-H) and hydroxymethyl metal compounds (MCH_2OH) [models for intermediates in the homogeneous hydrogenation of CO] are being carried out. Compounds with CH_3, CH_2, and CH groups bridging between two iron atoms have been synthesized as models for intermediates in the heterogeneous catalysis of CO hydrogenation. Carbon-carbon bond forming reactions of the CH compounds with alkenes and with CO are being explored. Several heterobimetallic compounds linked by a heterodifunctional ligand have been synthesized. Their reaction with hydrogen is being studied as a possible route to heterobimetallic dihydrides that might serve as catalysts for CO reduction. New compounds with directly bonded early and late transition metals have been synthesized and their fundamental chemistry is being explored; for example, $(C_5H_5)_2Zr[Ru(CO)_2C_5H_5]_2$ has been made and its reactions with CO and H_2 are under investigation.

347. *Acid Sites Formed By Doping Cations Onto Oxide Surfaces: Theoretical Aspects and Experimental Studies*

J.A. Dumesic, Dept. of Chemical Engineering **$61,200**

Our current research involves the characterization of acid sites formed by doping transition metal cations onto oxide surfaces. Our initial studies in this direction are focused on the use of iron as the dopant and irreducible oxides as supports (e.g., silica, magnesia, alumina). Adsorption of basic molecules is being used to probe the number of acid sites formed in this manner. Combined with infrared spectroscopy and temperature programmed desorption, this also provides information about the nature and the strength of the acid sites. One objective of our present studies is to relate the chemical properties of the acid sites to solid state structure. In this respect, Moessbauer spectroscopy is being used to determine the oxidation state and coordination number of the iron cations on the different oxide support surfaces after various catalyst pretreatments. We are assessing the catalytic consequences of our research using the decomposition of isopropanol as a catalytic probe reaction.

Wayne State University
Detroit, Michigan 48202

348. *Synthesis, Static, and Reactive Characterization of Supported Organometallics*

A. Brenner, Dept. of Chemistry **$83,000**

The nature and activity of catalysts derived from supported carbonyl complexes is being studied. The technique of temperature programmed decomposition has been applied to examine the nature of the bonding of $Mo(CO)_6$ to a variety of zeolites as a function of structure (A, X, Y, ZSM-5), Si/Al ratio, and cation identity (H^+, Na^+, Mg^{2+}) of a zeolite. The use of photolysis as an alternative to thermal activation is also being studied. Both $Fe(CO)_5$ and $Mo(CO)_6$ can be almost completely decarbonylated when supported on silica to produce a highly dispersed metallic catalyst. Exhaustive decarbonylation is not yet possible when supported on alumina. Catalysts produced by photolysis have been tested for the ability to equilibrate a H_2-D_2 mixture. The catalysts have very high activity for this reaction. Since the reaction is usually much faster on metal surfaces than on oxides or molecular complexes, it is a useful probe of the nature of the active sites on a catalyst. Structure-activity studies for benzene hydrogenation are also being developed. The analysis system for Fischer-Tropsch synthesis has been improved and it is now found that over $W(CO)_6Al_2O_3$ the rate of reaction is fifty-fold higher than that over a traditional catalyst (derived from WO_3) and the products are primarily methane, ethane, and propane.

Yale University
New Haven, Connecticut 06511

349. *Studies of the Hydrogenation of Small Unsaturated Molecules Using Organometallic Cluster Compounds As Catalysts*

R.D. Adams, Dept. of Chemistry **$23,800**
(3 mo.)

This research project is focused on the mechanisms of activation and hydrogenation of small heteronuclear unsaturated molecules like CO and CO_2 by polynuclear transition metal complexes. Special emphasis is being placed on the importance of multinuclear bridging coordination forms in ligand activation. The products of selected reaction sequences are being investigated by IR and NMR spectroscopies, and are being structually characterized by single-crystal x-ray diffraction analyses.

350. *Studies in Carbon Carbon Bond Activation*

R.H. Crabtree, Dept. of Chemistry **$70,000**
(8 mo.)

The aim of this research is to find ways of cleaving carbon-carbon bonds in alkanes and other related hydrocarbons with transition metal complexes. We believe that to do this we first have to break carbon-hydrogen bonds to give an organometallic species that can subsequently undergo a carbon-carbon bond cleavage. For example, we have shown that cyclopentanes can be dehydrogenated to cyclopentadienyl complexes by $IrH_2(solv)_2L_2$ cations. One proposal is to attempt the reaction with *gem*-dimethylcyclopentanes to see if a dimethylcyclopentadienyl complex can be obtained. This should subsequently undergo alkyl transfer to give a methyl iridium cyclopentadienyl complex. Other related strategies are discussed as well as possible extensions to catalytic systems ("homogeneous reforming").

351. *Selectivity, Activity, and Metal-Support Interactions of Rh Bimetallic Catalysts*

G.L. Haller, Dept. of Chemical Engineering **$80,000**

This research program is designed to investigate the effects of a modifying second metal and/or the support on the selectivity and activity of Rh supported catalysts. The systems of current interest are Rh/TiO_2, Rh/V_2O_3, and Rh-Pt bimetallics supported on SiO_2, Al_2O_3, and TiO_2. Rh-Pt is unique among the noble intergroup VIII bimetallic catalysts by virtue of the extremes of the activity of the individual components (for alkane hydrogenolysis and isomerization) and the potential for the formation of homogeneous bimetallic particles. The structure of the Rh bimetallic catalysts on various supports will be determined using XPS, EXAFS, NMR, and complementary chemisorption and catalytic test reactions. Among the catalytic test reactions will be hydrogenolysis, alkane isomerization, and CO/H_2 reactions.

352. *The Role of d-Electrons in Chemisorption and Metal Support Interactions Studied By Electron Spectroscopy*

V.E. Henrich, Dept. of Applied Physics **$60,000**

This research program utilizes model supported catalysts (small Rh particles desposited *in situ* on well characterized TiO_2 single-crystal surfaces) and surface-sensitive electron spectroscopies, including photoemission and Auger spectroscopy, to examine the role of d-electrons and support electronic structure in strong metal/support interactions. Core level binding energies of the Rh atoms measured by photoemission are found to depend upon particle size. The primary cause is believed to be changes in screening of the core hole, although changes in the valence state of the Rh atoms cannot be ruled out. Heating the model catalyst to 400°C results in a decrease in the amount of exposed Rh and supression of CO chemisorption. Inert gas sputter profiling of the catalysts before and after such reduction indicates that the Rh particles become partially covered by an oxide of Ti. Removal of the Ti oxides by inert gas sputtering restores CO chemisorption. The effects of various catalyst treatments are currently being investigated in order to correlate the electronic and geometric effects that have been observed to strong metal/support interactions.

353. *Energies of Organic Compounds*

K.B. Wiberg, Dept. of Chemistry **$88,000**

This research project is designed to provide information on the energies of organic compounds via reaction calorimetry and theoretical calculations, and to use these data to improve empirical and semi-empirical schemes for estimating the energies of these compounds. Heats of vaporization are being measured so that the thermochemical data may be corrected to the vapor phase. The data are also being used to explore steric effects and other structural effects on energies. Reactions being studied include the hydration of alkenes, hydrolysis of ketals, reduction of ketones, and rearrangements of small ring hydrocarbons. Theoretical calculations (RHF) are being used to estimate the energies of interesting compounds which have not as yet been prepared, and to study the intramolecular interactions (force constants and rotational barriers) and charge distributions which are used in molecular mechanics.

Separation and Analysis

Aerospace Corporation
EL Segundo, California 90245

354. *Laser Fluorescence Studies of Metallic Ions in Flames For Improved Detection*

F.E. Hovis, J.A. Gelbwachs, Chemistry & Physics Lab. **$27,800**

The use of fluorescence methods on neutral metal atoms in flames is a well established analytical technique. We propose to investigate laser induced fluorescence of metallic ions in high temperature flames for analytical applications. The first study involves the direct laser excitation of ionic fluorescence of the alkaline earth metals. A second experiment investigates neutral-ion energy transfer in metals as a means of sensitized ion fluorescence for multielement analysis. The use of sensitized ion fluorescence would allow simultaneous analysis of several metals using a single laser excitation line. The use of neutral-ion energy transfer is anticipated to yield superior detection limits to neutral-neutral energy transfer, and to have good potential as a practical analytical tool. These studies will yield information of both practical and fundamental interest.

355. *Isotopically Selective, Two-Step, Laser Photodissociation of Molecules*

P.F. Zittel, Chemistry and Physics Lab. **$115,000**

This research project is directed toward understanding those photophysical, energy transfer, and chemical processes relevant to isotope separation by two-step laser photodissociation of small molecules. The two-step technique involves the excitation of molecules containing a chosen atomic isotope to an excited vibrational state by an infrared laser, followed by ultraviolet laser photodissociation and scavenging of the photofragments. A computer-interfaced, dual beam, IR absorption apparatus is used to measure the absorption of intense IR laser pulses by the target molecule as a function of pressure and laser fluence. Mass spectrometric analysis of the photoproducts of the subsequent UV photodissociation step reveals the effect of vibrational excitation on the photodissociation cross section, and gives the isotope enrichments. Of particular interest are measurements of vibrationally state-specific photodissociation cross sections for different vibrational modes of a molecule. Two-step photodissociation of OCS has led to the separation of all stable isotopes of O, C, and S, and to a determination of the 249 nm photodissociation cross section of the ν_1 and $2\nu_2$ vibrational states of OCS. Rate constants for various vibrational energy transfer processes and chemical reactions are also inferred from isotope enrichment measures.

Bend Research, Inc.
Bend, Oregon 97701

356. *Fundamentals of Coupled-Transport Membranes*

D. Friesen, Division of Membrane Separation **$89,900**

The project objective is to study the fundamentals of coupled-transport membranes as applied to the concentration and separation of uranium and other metals. Coupled-transport membranes consist of a water-immiscible, liquid complexing agent held by capillary forces in the pores of a microporous polymeric support. This membrane separates two aqueous solutions of unequal concentrations. The complexing agent can pick up ions on one side of the membrane and carry them across the membrane by diffusion in the form of a neutral complex. Metal ions can be transported from a dilute to a concentrated solution by coupling their flow to that of another ionic species. The membranes are also selective due to the selectivity of the complexing agent toward one metal ion over other similar metal ions. Thus, coupled transport is of potentially practical value in hydrometallurgy, and in the treatment of radioactive wastes. Current efforts are focused on studying and improving the long-term performance of coupled-transport membranes. A model has been developed that is consistent with observed membrane performance. Based on this model, substantial progress has been made in developing membranes with commercially practical lifetimes.

Brigham Young University
Provo, Utah 84602

357. Separation of Selected Cations By Liquid Membranes

J.J. Christensen, Dept. of Chemical Engineering **$68,900**

Macrocycle-mediated cation transport using bulk, emulsion, and lipid vesicle liquid membrane systems is being investigated and modeled. In water-halocarbon-water bulk liquid membranes, transport is being studied of alkali and alkaline earth metal ions as a function of the halocarbon component and of Ag^+-K^+ mixtures where the relative Ag^+ and K^+ concentrations have been varied over a wide concentration range. The relative fluxes of cations from cation mixtures in water-toluene-water emulsion membrane systems is under investigation using the carrier dicyclohexano-18-crown-6, and various complexing anions in the interior receiving phase. The transport in these emulsion systems of amphoteric metals as anionic species coupled to a pH gradient across the membrane is also being studied. Dicyclohexano-18-crown-6 and other macrocycles have been incorporated into phospholipid vesicles as a means of making the vesicles selectively permeable to cations. The chemical and thermodynamic characteristics of the interaction, individually and as mixtures, of Pb^{2+}, Ca^{2+}, Sr^{2+}, and Ba^{2+} with these vesicles is being investigated.

Brown University
Providence, Rhode Island 02912

358. Photochemical Generation of the Optoacoustic Effect

G.J. Diebold, Dept. of Chemistry **$72,200**

Photochemical generation of the optoacoustic effect is being investigated. Chain reactions can be studied by recording the amplitude and phase of the optacoustic signal. As small amounts of different chemical species are added to systems undergoing photochemical chain reactions, the optacoustic signal is either enhanced or diminished according to the effect of the added species on the chain length and overall reaction exothermicity. Inhibitors act to shorten chain lengths which is observed experimentally as a dramatic reduction in the chemically amplified signal recorded in a lockin amplifier. It is possible to test different models of the mechanism of inhibitions by comparison of the experimental optoacoustic signal amplitude with the predictions of a kinetic model. The objective of this research is to investigate the optoacoustic effect with its inherent high sensitivity and unique response to energy release as a technique for chemical analysis.

Calspan Advanced Technology Center
Buffalo, New York 14225

359. Energy Transfer and Reaction Kinetics of Vibrationally Pumped Molecules

J.W. Rich, Dept. of Physical Sciences **$57,000**

This is a project for experimental and analytical research into energy transfer and reaction kinetics of vibration-to-vibration (V-V) pumped molecules. Extreme V-V pumped vibrational population distributions in CO, NO, and other gaseous species are produced by optical excitation. Special emphasis is being placed on isotopic enrichment reactions of V-V pumped CO, which yield products enriched in ^{13}C, ^{17}O, and ^{18}O. Processes limiting vibrational up-pumping in CO and NO are being studied, especially vibration-to-electronic energy transfer from the pumped ground electronic state of these molecules to low lying excited electronic states. The rate equation kinetic modeling of these processes is being developed.

Columbia University
New York, New York 10027

360. Utilization of Magnetic Effects As a Means of Isotope Enrichment

N.J. Turro, Dept. of Chemistry **$69,900**

This research project is directed toward the development of novel methods for the separation of isotopes, based on exploitation of differences in magnetic properties of isotopes. Emphasis has been placed on discovering reactions and conditions that allow the separation of isotopes which possess a finite magnetic moment from those which do not possess a magnetic moment. Successful systems have been designed for separation of ^{13}C (a magnetic isotope) from ^{12}C (a non-magnetic isotope), and for the separation of ^{17}O (a magnetic isotope) from ^{16}O and ^{18}O (non-magnetic isotopes). The restricted space provided by porous silica has proven to be an excellent environment for efficient separation of ^{13}C and ^{12}C based on the photolysis of dibenzyl ketone. The efficiency of enrichment as a function of pore size is being investigated. It should now be possible to design a practical system to separate these isotopes.

George Washington University
Washington, District of Columbia 20052

361. New High Temperature Plasmas and Sample Introduction Systems For Analytical Atomic Emission Spectrometry

A. Montaser, Dept. of Chemistry **$58,100**

New high temperature plasmas and new sample introduction systems are developed for rapid elemental analysis of solutions and solids using atomic emission spectrometry. These devices offer promise of solving singularly difficult analytical problems that either now or are likely to arise in the future in the various fields of energy generation, environmental pollution, biomedicine, and nutrition. Emphasis is being placed on: (1) generation and fundamental investigation of annular plasmas that are suitable for the excitation of high energy spectral lines, with the intent of enhancing the detecting powers for a number of elements; (2) generation of plasmas that require low gas flows and low input power, with the intent of decreasing the cost of analytical determination; and (3) development and characterization of new sample introduction systems that consume microliter or microgram quantities of samples. Investigations include the fundamental principles behind the measurements, the evaluation of the analytical potentials of the devices developed, and the demonstration of the analytical methods in representative samples.

Kent State University
Kent, Ohio 44242

362. *Adsorption and Desorption of Hydrocarbons At Low Concentrations*

R. Madey, Dept. of Physics **$71,000**

The aim of this research is to study the adsorption and diffusion of hydrocarbon gases through porous media adsorber beds. The approach involves calculations based on a mass-balance equation of the quantity of adsorbate adsorbed on an adsorbent, measurements of adsorption isotherms of hydrocarbons on activated carbon and polystyrene beads at selected temperatures, and studies of the dynamics of breakthrough curves with both a step-function and a pulse change of the input concentration. The breakthrough curves of binary mixtures exhibit interference phenomena where the output concentration of the weakly-adsorbed component increases above the input concentration until the other component elutes. An objective of this study is to provide a quantitative explanation of interference phenomena. The approach will be to obtain binary adsorption isotherms, to examine the mechanisms of intraparticle diffusion and longitudinal diffusion of the system, and to study the mathematical characteristics of the differential equation that governs the system.

National Bureau of Standards
Washington, District of Columbia 20234

363. *Competitive Ion Kinetics in Direct Mass Spectrometric Organic Speciation*

L.W. Sieck, Center for Chemical Physics **$131,000**

This research project involves the measurement of fundamental properties of gas phase ions, including fragmentation and reaction mechanisms and rates, structures, and the thermochemistry associated with ionization, protonation, and reaction. When appropriate, this information is then used to suggest chemical ionization techniques which incorporate competitive ion kinetics, and permit identification and/or assay of specific compounds or classes of compounds occurring in complex organic mixtures. The experimental project uses the NBS pulsed high pressure mass spectrometer system as the prime facility, and an ion cyclotron resonance instrument is also available. Work-in-progress includes determinations of enthalpies of protonation, hydration, and solvation of complex amines, ethers, and sulfur compounds, as well as systematic studies of the unimolecular kinetics associated with ion pyrolysis. Analogous measurements involving complex negative ions, particularly their thermal stability and reaction kinetics, are also currently receiving emphasis.

Purdue University
West Lafayette, Indiana 47907

364. *Reactions of Gaseous Metal Ions/Their Clusters in the Gas Phase Using Laser Ionization: Ion Cyclotron Resonance Spectroscopy*

B.S. Freiser, Dept. of Chemistry **$85,000**

A laser ionization source is used in conjunction with ion cyclotron resonance spectroscopy to generate and study the gas phase chemistry of simple metal ions and their clusters. Using this technique, metal ions are generated directly by focusing a high-powered pulsed laser onto the pure metal. The goals of this work have been threefold: (1) determination of fundamental reaction mechanisms and trends in reactivity; (2) comparison of gas phase to solution phase results; and (3) development of metal ions as selective chemical ionization reagents. These goals have been pursued thus far in extensive studies of Cu^+ with esters and ketones, on Fe^+ with ethers and ketones, and on Fe^+, Ti^+, Co^+, Ni^+, Rh^+, V^+, Y^+, and Sc^+ with hydrocarbons. In addition, work has been started on the effect of ligands on metal ion reactivity. Studies of $M\text{-}X^+$ ions, where $X = O$, S, CH_2, CH_3, and C_2H_4, for example, are well under way. This work has been catalyzed further with the acquisition of a Nicolet Fourier transform mass spectrometer (FTMS). Of particular importance is the application of collision-induced dissociation, using FTMS to elucidate ion structures and reaction mechanisms.

San Diego State University
San Diego, California 92182

365. *Development and Optimization of Methodologies For Analysis of Complex Hydrocarbon Mixtures*

R.J. Laub, Dept. of Chemistry **$65,000**

The goals of this project comprise exploration and further clarification of optimization methodologies for gas- and liquid-chromatographic separations of complex hydrocarbon mixtures. Emphasis is being placed at present on the kinetics of mass transfer, temperature effects, and mobile-phase composition in microbore- , conventional-bore, and rotating-disk thin-layer liquid-chromatographic techniques with silica, reversed-phase silica, and alumina adsorbents. Also being studied are metal-modified silica LC packings, including *in situ* generation, and alteration of the adsorbent surface. The utility of binary carriers in gas chromatography is being examined, where the second-interaction virial coefficients are predicted in advance from the McGlashan-Potter equation. Solute retentions are then calculated, where the separations achieved are a function both of the carrier pressure and composition. Work on establishment of a standard set of stationary phases for gas chromatography is being continued, where emphasis is being placed on newly-synthesized mesomorphic polysiloxane (MEPSIL) solvents.

State University of New York/Stony Brook
Stony Brook, New York 11794

366. *Fundamental Studies in Isotope Chemistry*

J. Bigeleisen, Dept. of Chemistry **$64,000**

Experimental and theoretical investigations are made of isotope effects in chemical and physical processes. When appropriate, applications are made to isotope separation processes and nuclear fuel cycles. Calculations have been made of the expected chemical properties of super-heavy isotopes of hydrogen, carbon, selenium, and uranium as a guide in the search for such particles. Detailed calculations have been made of the separation expected of superheavy isotopic forms of CO by fractional distillation. Relations between the isotope chemistry of oxygen and molecular structure are being studied. Regularities are found by an analysis of the effect of isotopic substitution on the entropies and enthaipies of formation of the compound from the gaseous oxygen atom.

367. Stable Isotope Studies

T. Ishida, Dept. of Chemistry **$81,600**

This project consists of basic studies of isotopic effects (IE) and applications to problems of stable isotope fractionation. With an aim at elucidating the nature of weak hydrogen bond-like interactions involving flourine atoms in the liquids, the anomalously large H/D-vapor pressure isotope effect (VPIE) and small $^{12}C/^{13}C$-VPIE in liquid methylene fluoride are correlated with intermolecular forces in the liquid, and they are compared with the VPIEs of other liquid fluoromethanes in the light of the extended cell model vibrational analyses and *ab initio* molecular orbital calculations. The $^{14}N/^{15}N$- and H/D-VPIEs measured for liquid and solid ammonia are analyzed to learn more critically about the nature of liquid ammonia, the material of importance in the heavy water production technology. Attempts are made to develop an ammonia-phobic heterogeneous catalyst for the H/D exchange between ammonia and hydrogen. The marked discrepancy between theoretical predictions and experiments on the pressure-dependence of the effective separation factor in the ^{15}N-enrichment system of nitric oxide/dinitrogen trioxide is investigated in the light of recent spectroscopic data. Based on the zero-point (ZPE) expansion obtained last year, additivity rules and contribution tables are developed for the IE in ZPE of various homologs.

Syracuse University
Syracuse, New York 13201

368. Mechanisms of Gas Permeation Through Polymer Membranes

S.A. Stern, Dept. of Chemical Engineering & Material Sciences **$75,000**

The objective of this study is to obtain a basic understanding of the mechanisms of gas permeation through nonporous polymer membranes. A free-volume model of gas permeation was found to describe satisfactorily the transport of many gases, and of a number of gas mixtures through polyethylene membranes. The model is applicable at temperatures above Tg, the glass transition of the polymer, over a wide range of pressures. The validity of the model is being tested with other polymer membranes. Simple correlations of free-volume parameters have been developed. These correlations permit the prediction of diffusion and permeability coefficients for many gases and components of gas mixtures. Solubility data are also required for this purpose. The gas permeation model has been extended to glassy polymers by incorporating in it the dual-sorption behavior observed below Tg. The extended model is being examined by means of time-lag and absorption-desorption measurements, with a number of gases in poly(n-butyl methacrylate) over a temperature range encompassing Tg.

369. Selective Metal Ion Extraction For Multiple Ion Liquid-Liquid Exchange Reactions

L.L. Tavlarides, Dept. of Chemical Engineering & Material Sciences **$77,000**

This research in hydrometallurgical solvent extraction is to develop a fundamental means to predict selectivity during simultaneous solvent extraction of multiple metal ions when kinetic rates and thermodynamic equilibria do not favor the desired metal. The chemical kinetics and thermodynamic chemical equilibria models for the system copper-iron acid sulfate solutions extracted by β-alkenyl-8-hydroxy quinoline-xylene system are being determined. A kinetic model for the initial forward rate of the iron extraction reaction is proposed. The model considers adsorption of HR, HR protonation, and that the formation of FeR_2 is the RDS. Kinetic data for the stripping reaction have been obtained and are being evaluated. Extraction experiments were conducted on a specially equipped 1-liter flow system with facilities for drop size measurements and *in situ* sampling of both phases for the iron system. A Monte Carlo simulation algorithm is employed to model droplet dynamics and predict extractor performance for the iron sulfate system as a function of system physico-chemical properties and operating parameters such as residence time, power input, dispersed phase fraction, and feed composition. The modeling includes aqueous phase equilibria and the reaction kinetics determined previously. Results suggest the validity of such models to predict extraction efficiencies of complex hydrometallurgical solvent extraction systems.

370. Particle Deposition in Granular Media

C. Tien, Dept. of Chemical Engineering & Material Sciences **$104,000**

This research is intended to obtain fundamental understanding of various phenomena arising from the flow of aerosol suspensions through, and the deposition of aerosols in granular media. The study is focused on the following areas: (1) experimental study of the transient state behavior of aerosol filtration in experimental filters; (2) the study of aerosol collection in magnetically stabilized fluidized filters and its modeling; and (3) the application of a specially designed two dimensional filter for *in situ* observation of the change of media structure due to the retention of aerosol particles.

Texas A & M University
College Station, Texas 77843-3255

371. Investigations On Multiphoton Ionization and Fast-beam Photodissociation Spectroscopy

D.H. Russell, Dept. of Chemistry **$90,000**

The emphasis of this research program is the development of combined laser-mass spectrometry methods for probing the dynamics of dissociation reactions. The experimental hardware and techniques are being developed using model chemical systems which have been characterized by other experimental methods (e.g., $C_6H_6^{+}\odot$, $C_4H_6^{+}\odot$, $C_4H_4^{+}\odot$, and so forth). Following these preliminary investigations, the experimental capabilities will be applied to chemical systems in which this approach provides unique or unusual capabilities. These latter studies emphasize the structural characterization of large molecular systems (1,000-10,000 a.m.u.). These large molecules are ionized using fast-neutrals (8-10 KeV Xe) and fast-ions

(8-10 KeV Cs^+) fast-atom bombardment (FAB) and secondary ion mass spectrometry (SIMS) directly from the solid state. Also, these latter studies will be performed using a high resolution tandem mass spectrometer (Kratos MS-50TA), with high mass range capabilities (3,000-5,000 a.m.u.) and a Fourier transform mass spectrometer (Nicolet FTMS-2,000).

Texas Tech University
Lubbock, Texas 79409

372. *Use of Functionalized Surfactants in Flame Atomic and Luminescense Analysis*
D.W. Armstrong, Dept. of Chemistry **$87,000**

Nine functionalized surfactants are to be used in this project to enhance the sensitivity and improve the selectivity of flame atomic spectrometry (FAS) and luminescence methods of analysis. Conventional bulk industrial surfactants such as sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB) have been used with some success in improving both methods (particularly luminescence). The mechanism by which these surfactants produce their effects has been the subject of some controversy. By using our first generation of specially designed surfactants, we hope to improve the sensitivity of the aforementioned techniques an order of magnitude over that now possible. Through these surfactants, one should be able to achieve a degree of selectivity (for these methods) approaching that of chromatography. Lastly, this study should remove any doubt as to the mechanism by which surfactants produce signal enhancements in FAS and provide additional information on the feasibility and mechanism of micelle mediated luminescence.

373. *Metal Ion Complexation By Ionic Crown Ethers*
R.A. Bartsch, Dept. of Chemistry **$112,500**

The goals of this research are the synthesis of lipophilic crown ethers with pendant ionizable groups and the application of these compounds for selective metal ion complexation. A variety of lipophilic ionizable crown ethers are being prepared in which the following structural features are systematically varied: (1) the size of the polyether cavity; (2) the number and types of ethereal oxygens in the crown ether ring; (3) the attachment site(s) for lipophilic groups; (4) the presence or absence of aromatic groups as polyether ring substituents; and (5) the type of ionizable group. The ionizable functions include carboxylic, phosphonic, and sulfonic acid groups. The efficiencies and selectivites of these lipophilic ionizable crown ethers in competitive solvent extraction, liquid surfactant (emulsion) extraction, and bulk liquid membrane transport of alkali metal, alkaline earth, and transition metal cations are being assessed.

374. *Novel Approaches to Ionic Chromatography*
P.K. Dasgupta, Dept. of Chemistry **$85,000**

The objective of this research is to develop analytical methodology for high resolution, high sensitivity chromatographic analysis of ions. The approaches being pursued include: (1) use of filament filled helical ion exchanger membranes and double annular membrane geometries for continuous ion exchange; (2) utilization of the Debye-Falkenhagen effect in high speed frequency swept conductance detection and unambiguous detection of the nature of the ion from a derivative plot; (3) use of multidimensional spectral array detectors in conjunction with reverse phase packings and chromogenic ligands as eluents for transition metal analysis; and (4) exploration of annular helical capillary columns for very high resolution chromatographic work. Currently, the major effort involves use of highly lipophilic ions as ion interaction reagents (IIR) injected into the chromatographic system as programmed pulses. The IIR are eventually completely exchanged by a helical membrane based exchanger.

University of Arizona
Tucson, Arizona 85721

375. *Chelating Extractants of Improved Selectivity*
H. Freiser, Dept. of Chemistry **$82,400**

This research is designed to develop chelating extractants of improved selectivity for separating individual lanthanide and actinide ions. Emphasis is on uncovering molecular structural parameters of importance in the design of such extractants. Use of pattern recognition techniques represents one approach to the elucidation of molecular parameters. Study of the extraction equilibria for representative tervalent lanthanides with selected members of chelating extractants of the N-acylphenylhydroxylamine, 8-quinolinol, acylpyrazolone, and other families is being used, both because they include some likely candidate extractants and because present gaps in fundamental data required to apply pattern recognition are thereby being eliminated.

University of California/Irvine
Irvine, California 92717

376. *Studies of Isotopic Mass Effects in Chemistry*
M. Wolfsberg, Dept. of Chemistry **$80,000**

This project deals with theoretical studies of isotopic mass effects on molecular properties. Such work is usually carried out within the framework of the Born-Oppenheimer approximation. Exact expressions for the complete quantum mechanical Hamiltonian operator of molecules are being constructed to study this approximation. Statistical mechanical calculations of isotope effects on a variety of molecular properties require a knowledge of rotational-vibrational energies of molecules and of isotope effects on these energies. Such energies are being calculated by the variational method for formaldehyde, water, and other molecules. The tunneling phenomenon and isotope effects on tunneling are being studied by an investigation of the vibrational energy levels of molecules with double-minimum potentials, in particular ammonia. Molecular dynamics calculations are being carried out on aqueous solutions of rare gases and of diatomic molecules such as nitrogen, to elucidate isotope effects on Henry's law constants as well as to study the structure of these solutions. The difference between gas phase and condensed phase infrared spectra is being studied in connection with isotope effects on vapor pressures.

University of California/Los Angeles
Los Angeles, California 90024

377. *Multiheteromacrocycles That Complex Metal Ions*

D.J. Cram, Dept. of Chemistry **$125,000**

This research involves the design, synthesis, and evaluation of cyclic and multicyclic organic compounds that selectively complex metal salts and solubilize them in organic solvents. Spherands are synthetic ligand systems that in the uncomplexed state contain enforced cavities lined with electron pairs. Rigid cyclic frameworks support attached heteroelements so that their unshared electron pairs occupy convergently arranged orbitals. Spherands are being studied whose cycles are composed of six to eight six-membered rings bonded to one another at their 1,3-positions, and which carry substituents in their 2-positions. Chorospherands are part crown and part spherand, and cryptospherands are part cryptand and part spherand. Spherands, chorospherands, and cryptospherands are being studied which contain anisyl, pyridine, pyridine oxide, benzoquinone, thioanisyl, cyclic urea, phenol, and benzenecarboxylic ester units. Complexes are designed with the help of CPK molecular models. Synthetic methods are then developed by which the ligand systems are prepared. The compounds are then tested for their metal ion-binding abilities and specificities.

University of Georgia
Athens, Georgia 30605

378. *Study of Mechanisms of Hydrogen Diffusion in Separation Devices*
M.H. Lee, Dept. of Physics and Astronomy **$77,000**

This study centers on separating hydrogen from mixtures of light gases by means of diffusion through metals. The hydrogen diffusion is highly selective, showing nonclassical behavior. The metal-hydrogen systems have mean-field critical dynamics. To describe the hydrogen diffusion, a quantum mechanical model is constructed, based on cluster formation. The diffusion is regarded as a collective movement of clusters. The sizes of these clusters depend on interatomic forces and particle statistics. The observed reversed isotope effect is explained by different degrees of cluster formation in hydrogen and deuterium. The diffusion constants are calculated by solving the generalized Langevin equation via the methods of recurrence relations recently developed by us.

379. *Fundamental Studies of Separation Processes*
L.B. Rogers, Dept. of Chemistry **$78,000**

There are three major areas of effort in this research. The first is concerned with the fundamental aspects of two different forms of liquid chromatography, adsorption and steric exclusion, especially with respect to interaction during a given separation. Non-porphyrin compounds of vanadium and nickel, and commercial mixtures of oligomers of polystyrene are ideal solutes for these studies, because each type of sample covers a wide range of molecular weights. A second area involves the identification of those non-porphyrin compounds using a variety of techniques. The third area is concerned with recycle chromatography, a promising approach to separations of isotopic species.

University of Houston
Houston, Texas 77004

380. *Mechanisms of Cake Filtration*
F.M. Tiller, M. Tadros, Dept. of Chemical Engineering **$160,000**

This project is aimed at developing the theory of particulate separation involving compressible, porous beds or sediments as found in filtration, centrifugation, and sedimentation. A key feature of the investigation involves close collaboration between the University of Houston and Martin-Marietta Laboratories. Generation of reliable data and integration of the areas of pretreatment, thickening, and separation are objectives of the research. A rough predictive method for calculating parameters involved in functions relating porosity and permeability to effective pressure has been developed. Quantities used in the correlations include particle size and shape, and degree of aggregation. An apparatus for simulating a continuous thickener by partially fluidizing a bed of fine particles has been developed. Initial cake structure of deposits as affected by surface charge, suspension concentration, and agitation are being studied in relation to resistance to flow. Pressure distributions are used to study flow mechanisms and fine particle migration. The theory of centrifugal filtration of compressible cakes has been developed.

University of Illinois
Urbana, Illinois 61801

381. *Theta Pinch Discharges For Solids Vaporization and Elemental Chemical Analysis*
A. Scheeline, School of Chemical Sciences **$66,000**

A pulsed, magnetically constricted plasma (theta pinch) is being used for elemental chemical analysis. A 0.5-1.0 kJ discharge with rise time 2 microseconds is employed to heat and compress a plasma of either argon or helium. Various sample forms are being tested, as there is interaction between the shape of the sample, plasma formation, and plasma/sample interaction. Spatially resolved spectra are being exploited to assist in resolving continuum and line background from analyte emission. Time resolution will also be performed. Our goal is to design a discharge system which can vaporize high melting solids, whether conducting or non-conducting, for matrix free determinations of elemental composition of the solids being studied. Because the plasma survives for only a few microseconds, only the surface of the sample is likely to be attacked by the discharge. Possibilities of controlling the depth of sampling and the area over which sampling occurs will be explored.

University of Minnesota
Minneapolis, Minnesota 55455

382. *Continuous Reaction Chromatography*
R. Aris, R.W. Carr, Dept. of Chem. Engineering and Materials Science **$70,000**

Continuous reaction chromatography is a method for carrying out chemical reaction with simultaneous chromatography of reactants and products in a single continuous flow reactor. This can be accomplished by providing relative motion between the chromatographic packed bed and the feedstream. Investigations of the rotating cylindrical annulus for both liquid phase reaction-solid adsorbent and gas-solid catalytic reactions have been completed. A detailed modeling study of the behavior of a countercurrent moving bed chromatographic reactor has also been done. Experimental tests of a laboratory-scale countercurrent moving bed reactor are being carried out. Analysis of reaction products is being done by conventional gas chromatography and the performance of the reactor is being compared with theoretical predictions. The simulation of countercurrency by switching the feed between fixed columns is currently being investigated both theoretically and experimentally.

383. Interfacial Chemistry in Solvent Extraction Systems

R.D. Neuman, Dept. of Forest Products **$85,000**

Laser light-scattering techniques, in addition to classical surface chemical methods, are being employed to investigate the interfacial behavior of extractant molecules and to further our understanding of the role of interfacial chemistry in solvent extraction systems. This program is a coordinated effort to correlate the interfacial properties of extractant films with mass transfer and coalescence rates. Studies examining the effect of pH and extractant (HDEHP) concentration on interfacial tension measurements are being extended to include other metal ions such as Na^+, Cu^{2+}, Co^{2+}, Ni^{2+}, and Fe^{3+} in addition to Ca^{2+}. At certain concentrations of Ca^{2+} and pH the plots of interfacial tension versus logarithmic bulk concentration of HDEHP are reminiscent of those for a surfactant forming aggregates in bulk solution. This phenomenon of aggregate formation is being examined by a low-angle laser light-scattering method. An interfacial rheometer is being constructed to study the interfacial viscosity of extractant films. Efforts presently are focused on mass transfer and distribution studies of the extraction of Ca^{2+} from aqueous solutions to a n-hexane phase by HDEHP. Attention is also directed toward examining the fine structure of interfacial films by electron miscroscopy.

University of Missouri
Rolla, Missouri 65401

384. An Extraction/Separation Process With Extreme Energy Efficiency

S. Friberg, P. Neogi, Dept. of Chemistry **$86,000**

The purpose of this investigation is to examine the phase equilibria involved in an extraction/separation process with extremely low energy demand. The process uses the temperature dependent transitions of colloidal association structures in systems of water/polyethlylene glycol, dodecyl ethers/aliphatic hydrocarbons to permit spontaneous extraction and separation with a temperature change of only 20°C. The main emphasis is placed on the role of liquid crystals to influence the kinetics of the extraction process.

University of Oklahoma
Norman, Oklahoma 73019

385. A Study of Micellar-Enhanced Ultrafiltration

J.F. Scamehorn, S.D. Christian, School of Chemical Engineering and Materials Science **$64,899**

In micellar-enhanced ultrafiltration, surfactant is added to aqueous streams containing dissolved organics. Aggregates called micelles are formed, into which a very high fraction of the organic solute tends to be distributed. The solution is then passed through an ultrafiltration filter with pores just small enough to prevent the micelles from passing through. Very little of the organic solute passes through the membrane, resulting in a fairly pure filtrate, and in the retentate solution being very concentrated in the solute. Cationic surfactants have been found to be superior to anionic or nonionic surfactants and, as a result, hexadecylpyridinium chloride is being used in this work. The model organic solute whose separation is being studied is tert-4-butylphenol. The accuracy of assuming that the filtrate and retentate are in equilibrium under expected operating conditions is being investigated. The severity of concentration polarization effects is being determined. Reductions in feed solute concentrations by a factor of 100 in the filtrate have been observed. Conditions to attain even further reductions are being sought.

University of Tennessee
Knoxville, Tennessee 37996-1600

386. Systematic and Structural Studies of Polymeric Extractants For the Separation and Recovery of Metal Ions

S.D. Alexandratos, Dept. of Chemistry **$81,400**

The research is directed toward the synthesis and evaluation of polymer-supported extractants, with emphasis on the properties of the polymeric support. Focus is on the development of polymeric extractants that will be commercially feasible for large-scale applications to the recovery of strategically important metals and within nuclear waste reprocessing plants. The study is concerned with four major points: (1) to develop an economical synthesis of the polymer support; (2) to utilize polymers that display high chemical, mechanical, and radiation stability; (3) to develop polymers with macroscopic properties allowing for a rapid rate of metal ion complexation; and (4) to produce polymeric extractants with a high density of active sites in order to minimize bed volumes. The principle polymer support examined to date is polystyrene, in bead form, at various levels of crosslinker and macroporosity. Bonding phosphinic acid moieties to the styrenic network yields a polymer-supported extractant found to absorb large levels of transition metal ions from aqueous solutions even at low pH values. Sulfonic acid and carboxylic acid groups bonded to the styrenic network are also being studied. Introduction of a higher level of selectivity is accomplished by the synthesis of polymer networks supporting both (pseudo)crown ethers and a cation exchange group.

387. Capillary Separations With Calorimetric Absorbance Detection

M.J. Sepaniak, Dept. of Chemistry **$61,400**

The objective of this project is development and utilization of laser-based calorimetric absorbance detection techniques in microscale liquid chromatography. A single beam configuration has been employed for a preliminary evaluation of thermal lens detection in open tubular liquid chromatography. Nitroaniline compounds were efficiently separated on 20 μm i.d. bonded-phase columns and detected with sensitiveities that rival fluorometric detection. A more versatile pulsed double beam configuration, exhibiting enhancements in sensitivity relative to Beer's Law of one-two orders of magnitude, was constructed. This thermal lens detector is being employed in the detection of nitropyrene compounds separated using μ-bore liquid chromatography columns. Procedures for reliably preparing bonded-phase open tubular columns are under investigation. Very good chromatographic efficiencies have been obtained for separations using open tubular columns prepared from soda-lime and borosilicate glasses. In addition, dynamically modified open tubular columns are being investigated for bioseparations.

University of Texas at El Paso
El Paso, Texas 79968-0513

388. *Macrocyclic Lanthanide Ion Selective Reagents*
C.A. Chang, Dept. of Chemistry **$50,000**

This research involves a topological approach for the design, synthesis, and characterization of macrocyclic lanthanide ion selective reagents. Macrocyclic aza-crown ethers, with pendent ionizable groups and a variety of structural features, are being prepared. Fundamental studies of their lanthanide complexes concerning thermodynamic and kinetic stabilities, solution and solid state structures, as well as the solvent extraction and liquid chromatographic behavior are being performed. Factors such as (1) the cavity size, and (2) the stereochemical constraint of the reagents are being examined to correlate to the selective complexation of lanthanide ions. Comparative complexation studies using other metal ions are also under way for eventual practical applications (e.g., to nuclear fuel and waste processing and the recovery of strategic metals).

University of Utah
Salt Lake City, Utah 84112

389. *Fourier Transform Photoacoustic Spectroscopy*
E.M. Eyring, Dept. of Chemistry **$75,000**

Microphonic photoacoustic spectroscopy (PAS) has proven to be a useful analytical tool for qualitative identification, and in favorable situations, quantification of chemical species adsorbed at a gas-solid interface or at shallow depths (< 1 mm) in the bulk solid. Numbered among the disadvantages of the technique are its unsuitability for detection of fast transient chemical species or work at high gas pressures and under vacuum plus the difficulty of microphonic measurements at elevated temperatures. Two other photothermal spectroscopies, photothermal beam deflection (PBD) and photothermal radiometry (PTR), have lately emerged that appear capable of circumventing these limitations. FT-IR/PBD spectral studies of organic polymers selected for their opacity and comparative chemical simplicity will be carried out over an extended range of temperatures and pressures. The objective will be the determination of the basic chemistry required for FT-IR/PBD spectroscopy to surpass FT-IR/PAS in usefulness. A byproduct of the resulting infrared spectral information will be an improved understanding of doping of semiconducting organic polymers. Some of the same polymer samples will be reexamined by PTR using pulses of near infrared radiation from a Raman shifted Nd:YAG laser to excite the sample and HgCdTe detectors to measure emitted radiation.

390. *Hydrophobic Character of Nonsulfide Mineral Surfaces As Influenced By Double Bond Reactions of Adsorbed Unsaturated Collector Species*
J.D. Miller, Dept. of Metallurgy and Metallurgical Engineering **$75,000**

The separation of nonsulfide minerals from ore is frequently accomplished by froth flotation using unsaturated fatty acids as collector. Variables such as temperature, oxygen partial pressure, and solution chemistry have a significant effect on flotation rate and the hydrophobic character of non-sulfide minerals. Bubble attachment measurements indicate that attachment times decrease by an order of magnitude at higher temperature and higher oxygen partial pressure when compared to ambient conditions. These results suggest interaction of unsaturated chemisorbed carboxylate species, which may involve oxidation of the double bond and subsequent cross linking between adjacent unsaturated chains. The hydrophobic character of such surfaces is being studied by collector adsorption density measurements, microcalorimetric studies, and *in situ* FTIR spectroscopy. *In situ* spectroscopic experiments are being performed to identify the surface reaction product and establish whether or not oxidation of the double bond and polymerization of the chemisorbed species occurs at non-sulfide mineral surfaces. If such a reaction is operative, the implications are far-reaching. Catalysts or new collectors can be developed to improve the performance, selectivity, and energy-economy in nonsulfide mineral flotation systems.

University of Virginia
Charlottesville, Virginia 22901

391. *Glow Discharge As An Atomization and Ionization Source*
W.W. Harrison, Dept. of Chemistry **$64,899**

This project centers about the study of a glow discharge as an atomization and ionization source for trace element analysis of solids and solutions. Coupling of the glow discharge to a quadrupole mass filter results in a simple mass spectrometer system of considerable versatility. A variable duty pulsed discharge is being studied, and shows advantages over direct current operation. The use of short, high intensity pulses produces enhanced sputter action and a greater ion yield. Time-resolved selection of ions generated only during the trailing pulse edge produces a strong atomic signal for the cathode sample with discrimination against background gases. The use of laser enhanced ionization within the glow discharge is also under investigation. Resonance transitions stimulated by tuned radiation from an excimer/dye laser permit selective ionization of sputtered metal atoms. Up to 100% of the selected atoms in a given microvolume can be ionized for subsequent mass spectral analysis.

University of Wyoming
Laramie, Wyoming 82071

392. *Solid Surface Luminescence Analysis*
R.J. Hurtubise, Dept. of Chemistry **$77,400**

The goal of this project is to develop a fundamental understanding of the physical and chemical interactions that induce strong room-temperature fluorescence and phosphorescence from organic compounds adsorbed on solid surfaces. Reflectance, infrared, and luminescence spectroscopy are being used to clarify the interactions. The effects of moisture, several gases, and temperature on the luminescence quantum efficiencies and the phosphorescent lifetimes of adsorbed compounds are being investigated. The various experiments will help to determine if the luminescent molecules are being held rigidly, or if the solid matrix is preventing collisions with oxygen and water molecules. Basic and nonbasic nitrogen heterocycles, and hydroxyl aromatics are being used as model compounds to develop total luminescence derivative spectroscopy as a new approach in organic trace analysis. In addition, cyclodexdrins are being used to induce room-temperature luminescence from adsorbed compounds. Finally, solid-surface luminescence is being employed to study interactions in adsorption chromatography.

Washington State University
Pullman, Washington 99164-4630

*393. **Studies of the Analyte-Carrier Interface in Multicomponent Flow Injection Analysis***
S.D. Brown, Dept. of Chemistry **$75,000**

The use of flowing carrier solutions to transport injected analytes to a detector has received considerable attention recently. Situations where the injected analyte reacts with reagents present in the carrier have received almost no study, on the other hand. Analyte-carrier reagent interactions are controlled by several factors. Among these are dispersion of analytes and carrier solutions, reaction kinetics of carrier reagents with components of the analyte solution, and the relative availability of reactants at the analyte-carrier reagent interface. This project involves the study of product distributions at the analyte-carrier reagent interface as a function of dispersion, reaction kinetics, and local stoichiometric effects. For these studies, a rapid-scan electrochemical flow detector is used to obtain "maps" of reaction product distributions at the analyte-carrier reagent interface. The added information obtained in probes of these distributions is useful in the design of species-specific analyses and multicomponent analyses using flowing solutions.

Chemical Engineering Sciences

Brigham Young University
Provo, Utah 84602

*394. **Thermodynamic Study of CO_2-Organic Compound Interaction At High Pressures and Temperatures***
R.M. Izatt, J.J. Christensen, Dept. of Chemical Engineering **$71,900**

The primary objective of this project is to gain increased knowledge of the energetics associated with the interaction of CO_2 and Freons with selected organic compounds under temperature-pressure conditions where either one or more of the components is in its super-critical region. The quantities measured include heats of mixing of binary and ternary mixtures and constant pressure heat capacities of pure components and of mixtures. The temperature and pressure ranges covered are 285-673 K and 8-12.5 MPa, respectively. Flow calorimeters will be used to obtain the experimental data. The data will be incorporated into equations which will describe the variation of each quantity over the temperature and pressure ranges studied. The eventual goal is to elucidate the chemistry occurring when supercritical fluids are involved in solvent extraction processes.

California Institute of Technology
Pasadena, California 91125

*395. **Dynamics of Vapor Explosions***
B. Sturtevant, Graduate Aeronautical Laboratories **$46,000**

The effect of ambient pressure on the baroclinic interfacial instability of rapid vaporization has been studied experimentally and theoretically in single droplets boiling explosively at the limit of superheat. In a series of experiments with pentane, isopentane, and ethyl ether in a bubble-column apparatus it has been shown that the instability of super-heat-limit boiling may be suppressed by increasing the ambient pressure. While at atmospheric pressure bubble boundaries are rough and opaque due to small-scale instability-generated distortions, at elevated pressure the liquid-vapor interface is smooth and transparent. The radiated pressure field is two orders of magnitude smaller from stabilized bubbles than from unstable. In the stable boiling regime the largest radiated pressures are a consequence, not of boiling, but of violent bubble oscillations that occur after the droplet has completely vaporized. At intermediate pressures bubble growth occurs in two stages, first stable, then unstable. The Landau mechanism for the instability of laminar flames has been adapted to the case of vaporization by accounting for the effects of surface tension and acceleration. A formulation of the theory in spherical geometry predicts absolute stability at atmospheric pressure, while the theory for planar interfaces yields results in accord with observation. Apparently, the instability occurs at such small wavelengths that the spherical constraint is inappropriate.

City College of New York
New York, New York 10031

*396. **Turbulence and the Distortion of Reactions***
J.A. Johnson, Dept. of Physics **$80,000**

Contact surfaces in a pressure-driven shock tube are used as a way of investigating the possibility of the manipulation of molecular recombinations. Turbulent bursts are produced. The reaction $2NO_2+X \rightarrow N_2O_4+X$ ($X = N_2$ or Ar) is unstable under some circumstances; fluctuations with amplitude incoherence and phase coherence are developed. Here, the use of standard reaction rate data proves to be inadequate. The point-resolved histories of density, velocity, and other flow and mixture properties are determined, using cross-beam correlations and fluorescence of NO_2 probed by the 4.88 nm line from an Ar^+ ion laser. The importance of the dynamical parameters of turbulence is being measured; specifically, the impact of changing local viscosity, characteristic turbulence scale, and turbulence intensity. In addition, there is some evidence that a reduced molecular chaos may be relevant to this kind of process. This possibility is given a quantitative formulation and tested in our data.

Columbia University
New York, New York 10027

397. Interaction of Turbulence and Chemical Reactions
R. Chevray, Dept. of Mechanical Engineering **$85,000**

Flow in a two-dimensional mixing layer is utilized to study a well-known reaction with simple kinetic scheme. The flow represents a well-defined turbulent situation, and additional complexities of finite heat release are avoided by use of small concentrations for the reaction chosen ($NO + O_3 \rightarrow NO_2^* + O_2 \rightarrow NO_2 + h\nu + O_2$). Large Reynolds numbers, small dilution numbers, large reaction speed numbers, and several concentration ratios are investigated. Conditional and conventional measurements are made of mean and fluctuating quantities for both the velocity and concentration fields by laser Doppler anemometry and absorption spectroscopy, respectively. Simultaneous cine-film recording is conducted, in order to determine the convection velocity of the interface and hence the entrainment. Numerical simulation is set up to model directly the equations describing the evolution of the species concentration in the shear layer.

Cornell University
Ithaca, New York 14853-0294

398. Experimental and Theoretical Studies of Dense Fluid Mixtures
W.B. Streett, K.E. Gubbins, School of Chemical Engineering **$180,000 (24 mo.)**

The primary goals of this research are: (1) to carry out wide-ranging thermophysical property measurements for pure fluids and mixtures; and (2) to develop improved methods for correlating, extrapolating, and predicting dense fluid properties using statistical mechanics and intermolecular potential theory. Experimental research in progress includes measurements of the PVT properties of CF_4 and CHF_3 at pressures to 1000 bars. The direct-weighing PVT apparatus, designed and built under this project, has been completely redesigned and reconstructed to extend the temperature and pressure ranges to 0-600 C and 0-2000 bars, respectively. Measurements of the velocity of sound in fluids over wide ranges of pressure and temperature will be initiated in 1984-1985. Theoretical work has included development of statistical mechanical methods for calculating the effects of molecular polarizability, including complicated multibody induction effects. These effects have been found to be almost an order of magnitude larger than anticipated on the basis of dilute gas calculations.

Hokenson Company
Los Angeles, California 90005

399. Coherent Structure: Reflective Turbulence Modeling of Complex Shear Flows
G.J. Hokenson, Fluid Mechanics and Heat/Mass Transfer Division **$20,000**

The limitations of turbulence modeling with respect to the accurate prediction of complex shear flows will be analyzed. The flowfield effects of interest are associated with combustor flows and include strong: (1) pressure gradients; (2) streamline curvatures; and (3) density gradients. Each effect will be considered alone and in combination with others to isolate the modeling implications regarding: (1) basic turbulent structures; (2) gradient transport; and (3) isotropy. Of particular interest is the strong turbulence suppression or enhancement which each effect may induce, involving the possible generation of dispersive wave-like features with a corresponding non-diffusive and highly anisotropic nature. The project objective is to provide a framework for future research in which successful turbulence modeling prescriptions may be carried over to a multiple-fluctuating-element representation of the flow. In such a formulation, the physics of processes occuring at various scales and coherences may be differentiated from each other and depicted in a manner faithful to the experimantal data. The practical utility of such an approach in providing accurate predictions of untested flows would then be tested.

Johns Hopkins University
Baltimore, Maryland 21218

400. Prediction of Thermodynamic Properties of Coal Derivatives
M.D. Donohue, Dept. of Chemical Engineering **$81,000**

The purpose of this project is to develop an equation of state to predict the thermodynamic properties of coal derivatives. The equation is based on perturbed hard-chain theory, but includes additional terms for multi-pole interactions. The equation allows prediction of vapor pressures, densities, and solubilities for a wide range of organic molecules including multiringed aromatics. Pure component and mixture parameters are determined from experimental data when available; a group-contribution correlation is being developed to allow prediction of parameters for systems where no experimental data are available. The applicability of the new equation to supercritical fluid extraction is being studied. Hydrogen bonding effects are being taken into account to predict properties of systems containing H_2O, alcohol, and so forth. High pressure vapor-liquid equilibrium measurements for CO_2- aromatic binary mixtures are being made.

National Bureau of Standards
Boulder, Colorado 80303

401. Experimental and Theoretical Study of the Thermophysical Properties of Fluid Mixtures
H.J.M. Hanley, Fracture and Deformation Div. **$205,000**

The program combines experiment, theory, and correlation to study the properties and behavior of fluids. Specific objectives are to produce PVT and thermodynamic data on hydrocarbon fluids and their mixtures at high temperatures (to 900 K) and pressures (to 35 MPa, possibly to 100 MPa) so as to (1) develop the theory of liquids, and (2) develop models to predict the properties based on the theory and optimized by the data. PVT properties of H_2S and propane have been measured and correlated. Phase equilibria VLE measurements of the system CO_2/i-butane have been reported. Theoretical studies include computer simulation of fluids under shear for which several results have been published. A thermodynamics for a shearing system has been proposed. Predictions of shear induced phase transitions in liquid/gas and liquid/liquid mixtures have been discussed. Plans include PVT studies of methanol and further computer simulation studies of mixtures.

402. *Transport and Phase Equilibria in Multicomponent Fluids*

J.M. Kincaid, Division of Thermophysics **$70,000**

The purpose of this project is to develop and implement simple, accurate techniques to treat the transport and phase transition properties of multicomponent systems. There are three basic aspects to the project: (1) the development of new techniques to study multicomponent systems; (2) the translation and adaptation of recent theoretical advances in transport and phase transition phenomena to forms usable to the energy technologies; and (3) approximation assessment and implementation. All three of these areas can be expected to advance our understanding of multicomponent fluids at high temperatures. Recent progress includes: (1) the solution of several phase equilibria problems for polydisperse fluids; and (2) an analysis of molecular dynamics studies of diffusion in binary hard-sphere mixtures, which will be used to calibrate the revised Enskog theory.

Purdue University
West Lafayette, Indiana 47907

403. *Gas-Liquid-Liquid Equilibria in Mixtures of Water, Light Gases, and Hydrocarbons*

K.C. Chao, H.M. Lin, School of Chemical Engineering **$75,000**

Phase equilibrium in mixtures of water + light gases, and water + heavy hydrocarbons will be investigated in light of recent advances of group contribution, equation of state, and local composition. Toward the development of quantitative models of water solutions, experimental study will be made of gas-liquid equilibrium at temperatures up to 430°C and pressures to 300 atm, and of liquid-liquid equilibrium at temperatures up to 250°C.

Stanford University
Stanford, California 94305

404. *Transport Characteristics of Slurries in Pipelines: Flow Regimes and Pressure Drop*

A. Acrivos, Dept. of Chemical Engineering **$0 (No Fund Extension)**

This research aims to study the flow of slurries in pipelines from a fundamental point of view. Primary emphasis is on developing methods, based on sound scientific principles, for predicting the pressure drop, and for delineating the various flow regimes that can occur in such systems. The theoretical framework is based on the equations of contiuum mechanics, and is being developed in close conjunction with a parallel experimental study. A theoretical model is currently being developed to explain quantitatively the curious phenomenon whereby a settled suspension has been observed to resuspend in the presence of a laminar shear flow under conditions of very small Reynolds numbers. It is believed that resuspension is due to the action of a shear-induced diffusion of particles, and attempts currently are being made to measure the corresponding diffusion coefficient. The possible connection between the shear-induced diffusion and the measured normal stresses in the suspension is being investigated.

405. *Fundamental Studies of Heat Transport, Fluid Mechanics, and Stability in Porous Media*

G.M. Homsy, Dept. of Chemical Engineering **$84,800**

This program treats problems in flow and transport phenomena in porous media whose solutions are of interest in energy recovery processes. Broad categories of activities include macroscopic and microscopic descriptions. Regarding the former, theoretical and experimental studies of the effect of graded mobility on instabilities of displacement fronts have continued. The theory is being extended to study important effects of flow-induced dispersion, and adsorption loss of the mobility control agent. Experiments in a Hele-Shaw cell are continuing, and to date have shown the stabilization of displacements due to mobility gradation. A theory of finite-amplitude thermally driven instabilities in bounded porous regions has been completed, which determines the form of convection which will be observed. Microscopic studies of two phase Hele-Shaw flows have been completed with good agreement between theory and experiment. Microscopic modeling of non-Newtonian flow in porous media has been studied, indicating that constitutive equations of the Oldroyd type are incapable of capturing the salient experimental features of these flows. New studies of blob dynamics in constricted-tube models of porus media have begun.

State University of New York/Stony Brook
Stony Brook, New York 11794

406. *Transport Properties of Multiphase Systems*

G.R. Stell, Dept. of Mechanical Engineering **$165,000 (24 mo.)**

Ongoing research continues on the microscopic theory relating transport and structure in two-phase media, including new results on expected surface area, and on quantitative comparisons of bounds and approximations that involve two-particle and three-particle correlations in such media. Research also continues on new statistical mechanical theories of transport at both liquid-state and gaseous-state densities. The liquid-state work includes the use of an entropy-maximization technique as well as a molecular theory of solutions and suspensions. Both approaches lead to new quantitatively useful approximations for transport coefficients in the liquid state. The gaseous-state work includes the development of analytically tractable kinetic perturbation theories for useful model potentials. A kinetic approach to the theory of mixtures of interacting n-mers has yielded new, exact results in the description of the gelation point, and the post-gelation period for models that include and go beyond that of the Flory-Stockmayer theory.

University of California/Davis
Davis, California 95616

407. *Statistical Modeling and Analysis of Chemically Reacting Turbulent Flows*

H.A. Dwyer, W. Kollmann, Dept. of Mechanical Engineering **$145,000 (24 mo.)**

This research program is directed toward development of new turbulent closure models for variable density turbulent flow and turbulent diffusion flames. The methods utilized to accomplish these goals are (1) physical and mathematical modeling, and (2) sensitivity analysis. The modeling techniques cover the closure of density-velocity statistical correlations and the use of Monte Carlo simulations for scalar transport. The research has centered on turbulent jets, but a new effort on boundary layer flows has been initiated. Sensitivity analysis studies have been extended to variable density and combustion flows; the results are giving insight into the complex interaction between combustion and turbulent flow.

University of California/Santa Barbara
Santa Barbara, California 93106

408. Reaction Enhancement of Heterogeneously Catalyzed Reactions By Concentration Forcing

R.G. Rinker, Dept. of Chemical and Nuclear Engineering **$57,800**

An investigation is under way to examine experimentally the underlying phenomena leading to enhancement of heterogeneously catalyzed reaction systems by periodic concentration cycling of reactants (concentration forcing). Several consequences of periodic cycling, compared to conventional steady-state operation for reactions with nonlinear pathways, include (1) higher time-averaged product yields, (2) longer catalyst life, (3) improved catalytic selectivity, and (4) lower energy costs. The results of this study, which is focusing on the synthesis reactions of ammonia and menthanol, are expected to provide new insight into how surface concentrations of reactants on catalysts can be manipulated under conditions of practical interest to kinetically accelerate the rate-limiting step(s) in the overall conversion. The results are also expected to provide new directions for catalyst design. Kinetic and thermodynamic parameters of the selected reactions, for use in modeling unsteady-state operation, are obtained in a differentially-operated fixed-bed reactor by transient experiments capable of distinguishing among individual phenomenological steps. Mathematical simulations of integral fixed-bed reactors having plug flow or perfect mixing in the fluid phase and operated under periodic cycling conditions (either isothermally or adiabatically) are being used to compare alternate inlet conditions including pulse widths, frequencies, and compositions. Results of the simulations are being compared to the experiment.

University of Pennsylvania
Philadelphia, Pennsylvania 19104

409. Thermodynamics of Systems of Very Many Components

E.D. Glandt, Dept. of Chemical Engineering **$79,900**

The purpose of this research is to develop a quantitative description of fluid mixtures of very many components by using a continuous distribution of an arbitrarily chosen parameter. The continuous or polydisperse Lennard-Jones fluid, where the molecular parameter is the distributed variable, is being studied first since it is an appropriate representation of hydrocarbon systems. The thermodynamic properties of this model mixture are studied by two complementary approaches: (1) Monte Carlo computer simulations; and (2) perturbation theory. In the perturbation theory calculations the reference fluid is the pure most abundant component while the small, perturbing parameter is the second moment or "width" of the composition distribution function.

University of Washington
Seattle, Washington 98195

410. Experimental Determination of the Mixing Frequency Parameter For Coalescence/Dispersion Modeling of Turbulent Combustion

G.W. Butler, Dept. of Mechanical Engineering **$70,000**

The purpose of this experimental study is to advance the understanding of the physics and physical modeling of turbulent mixing in high intensity combustion. Specific objectives of this research are: (1) to measure the characteristic fluid-mixing frequency in a jet-stirred reactor over a range of practical fuel-air equivalence ratios using time-resolved stimulus-response techniques; (2) to compare the experimental data with existing analytical and numerical models for combustor mixing frequencies which are derived from global fluid mechanical arguments; and (3) to interpret the measurements in order to model the dependence of the characteristic mixing frequency on the physical parameters of the high intensity combustion. From this study, physically based models of turbulent mixing frequencies which characterize high intensity combustion are expected. It is furthermore anticipated that these models will be used to extend the predictive and potential design utility of numerical coalescence/dispersion modeling of turbulent combustion processes.

FY 1984 EQUIPMENT FUNDS

Outlay funds of the Office of Basic Energy Sciences are divided among operating, equipment, and construction funds. Equipment funds are provided primarily to DOE laboratories. (Operating funds provided to other contractors are used for all costs, including purchase of necessary equipment.) Chemical Sciences FY 1984 equipment funds were assigned as follows:

Facility	Equipment funds
Ames Laboratory	447,000
Argonne National Laboratory	1,105,000
Bartlesville Energy Technology Center	15,000
Brookhaven National Laboratory	1,491,000
Idaho National Engineering Laboratory	11,000
Lawrence Berkeley Laboratory	1,071,000
Lawrence Livermore National Laboratory	0
Los Alamos National Laboratory	64,000
Mound Facility	71,000
Notre Dame Radiation Laboratory	252,000
Oak Ridge National Laboratory	691,000
Pacific Northwest Laboratory	116,000
Pittsburgh Energy Technology Center	7,000
Sandia National Laboratories, Albuquerque	58,000
Sandia National Laboratories, Livermore	800,000
Solar Energy Research Institute	65,000

SPECIAL FACILITIES

The special facilities described on the following pages are supported wholly or partly by the Division of Chemical Sciences. They represent an assembly of unique and/or expensive equipment which would be costly to develop elsewhere. They represent research resources for the general scientific community, and qualified scientists from laboratories outside the host laboratory are encouraged to make use of them. However, any activity that can be carried out through commercially available laboratories is not appropriate for these DOE supported facilities.

The process by which an off-site scientist can use a facility is discussed in each facility summary. For the National Synchrotron Light Source and the Combustion Research Facility, see the section "User Mode." For the remaining facilities, see "Collaborative Use," which is a process based on the need for collaboration by the off-site scientist with one or more in-house staff members.

Each of the facility summaries also gives the names of individuals to contact for further information, a general description of the facility, and a list of technical data on the primary available instrumentation.

The Office of Basic Energy Sciences also supports other facilities not summarized here. Information concerning these can be obtained by contacting Dr. Louis C. Ianniello, Director of Materials Sciences, ER-13, U. S. Department of Energy, Washington, D.C. 20545.

Chemistry Division
Argonne National Laboratory
Argonne, Illinois 60439

ATOMIC SPECTROSCOPY FACILITY

The Argonne spectroscopic facility is designed for high-resolution investigations of atomic and molecular optical spectra by using a unique combination of large-scale dispersive instruments with state-of-the-art holographic gratings and pulsed, sharply tunable coherent light sources for excitation energies of up to 11 eV. Photographic, Reticon array, and resonance-ionization detectors with associated data-processing equipment are available for a wide variety of experiments. Peripheral equipment includes a 50-kG superconducting magnet with a 24-inch room-temperature bore, high-temperature furnaces for metal-vapor absorption tubes, and an automatic plate-measuring comparator. YAG-laser-driven dye lasers are used with doublers and H_2-Raman scattering to cover the 2500- to 8500-Å range and to produce coherent radiation between 1180 and 1250 Å by four-wave mixing in mercury vapor at fluxes ranging from 10^{10} to 10^{16} photons/sec for resolving powers of several million. The experimental work is reinforced by extensive computational programs for interpreting line broadening, diamagnetic, and hyperfine structure data in terms of fundamental atomic theories.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists.

PERSON TO CONTACT FOR INFORMATION

J. P. Hessler
Chemistry Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Phone:
Comm. (312) 972-3717
or FTS 972-3717

TECHNICAL DATA

Resolving power	
30-foot Paschen-Runge spectrograph	$>5 \times 10^5$
5-meter Czerny-Turner spectrograph	$>10^6$
Tunable dye lasers	$>10^6$
Vacuum-ultraviolet coherent source	$>10^7$
Wavelength range, A	
30-foot Paschen-Runge spectrograph	2000 to 9000
5-meter Czerny-Turner spectrograph	1200 to 9000
Tunable dye lasers	2500 to 8500
Vacuum-ultraviolet coherent source	1180 to 1250

406

Physics Division
Argonne National Laboratory
Argonne, Illinois 60439

4.5-MV DYNAMITRON ACCELERATOR

The Argonne Physics Division operates a high-current 4.5-MV Dynamitron accelerator which delivers magnetically analyzed beams of most atomic ions and many molecular ions. Among the facilities associated with the Dynamitron are (1) a beam line capable of providing "supercollimated" ion beams that permit angular measurements to accuracies of 0.1 mrad, (2) a beam-foil spectroscopy setup with associated high-resolution photon (optical and X-ray) spectrometers, (3) a 28-inch-diameter general-purpose scattering chamber, (4) a simultaneous irradiation system by which ion beams from the Dynamitron and from a 2-MV Van de Graaff accelerator are focused onto the same target, (5) a variety of electron spectrometers including a high-resolution, large solid-angle McPherson spherical analyzer, and (6) a post-acceleration chopper system giving beam pulses with widths that can be varied from 1 nsec to several msec at repetition rates variable up to 8 MHz. A PDP-11/45 computer system with a direct link to Argonne's central computing facility is used for online data acquisition, analysis, and the control of experiments.

COLLABORATIVE USE

Visiting scientists use the accelerator either in collaboration with Argonne investigators or as independent groups.

PERSON TO CONTACT FOR INFORMATION

D. S. Gemmell
Physics Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Phone:
Comm. (312) 972-4004
or FTS 972-4004

TECHNICAL DATA

Range of terminal voltages attainable	0.3 to 4.5 MV
Range of ion beam currents attainable	0.1 nA to 100 A
Monatomic singly charged ion beams available	Most elements
Monatomic multiply charged ion beams available	Rare gases, transition metals
Typical molecular-ion beams available	H_2^+, H_3^+, HeH^+, CH_n^+ ($n = 1,4$), OH_n^+ ($n = 1,3$), CO^+, O_2^+, etc.
Pulse mode (post-chopper)	
Pulse width	1 nsec to 10 msec
Repetition rate	1 MHz to 8 MHz

Chemistry Division
Argonne National Laboratory
Argonne, Illinois 60439

PREMIUM COAL SAMPLE PROGRAM

The purpose of the Premium Coal Sample Program is to provide the coal science research community with long-term supplies of a small number of premium coal samples that can be used as standards for comparison. The premium coal samples produced from each coal and distributed through this program will be as chemically and physically identical as possible, will have well-characterized chemical and physical properties, and will be stable over long periods of time. Coals will be mined, transported, processed into the desired particle and sample sizes, and packaged in environments as free of oxygen as possible while maintaining the natural moisture content in order to ensure that the coals will be in as pristine and stable a condition as possible.

AVAILABILITY

Initial samples are expected to be available in early 1984. Samples will be made available to research personnel at a nominal replacement cost. A very limited quantity of lump coal, stored under similar inert conditions, will be available on special request for special physical property measurements. Distribution of these samples will be guided by policies established with the help of a users advisory committee. The processing facility may be available for occasional processing of special samples.

PERSON TO CONTACT FOR INFORMATION

Dr. Karl S. Vorres
Chemistry Division, Bldg. 200
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

Phone:
Comm. (312) 972-7374
or FTS 972-7374
Telex:
TWX 910-258-3285
USDOE-CH ARGN

Chemistry Division
Argonne National Laboratory
Argonne, Illinois 60439

PULSE RADIOLYSIS FACILITY

The Argonne linear electron accelerator was designed for chemical research. The moderate energy of the electron accelerator (21 MeV transient mode, 14 MeV steady state) allows the use of the electron beam for the generation of transient species without nuclear activation. The pulse width can be varied from 25 psec to 10 μsec. In liquids, transient concentrations up to 20 μ*M* can be generated with the 25-psec pulse, and concentrations in excess of 10 m*M* can be generated with the longest pulse. Instrumentation for measurement of chemical processes allows kinetic spectrophotometric absorption and emission and fast conductivity measurements. Simultaneous multiwavelength kinetic spectrophotometric measurements are possible, and very high time resolution measurements that use the short pulse capability of the linac can also be made, both in absorption and emission. Other detection techniques, such as resonance Raman spectroscopy, are under development. All data acquisition equipment is computer interfaced to provide accurate data reduction. Sample preparation and handling facilities are available for solid, liquid, and gaseous samples.

COLLABORATIVE USE

Collaborative experiments can be arranged with appropriate staff scientists.

PERSON TO CONTACT FOR INFORMATION

Charles D. Jonah Chemistry Division Argonne National Laboratory 9700 South Cass Avenue Argonne, Illinois 60439	Phone: Comm. (312) 972-3471 or FTS 972-3471

TECHNICAL DATA

Energy	
Transient mode	21 MeV
Steady-state mode	14 MeV
Pulse repetition rate	Single pulse, 800 pps (800 pps not possible for all pulses)
Current/pulse	
Transient mode	20 A
Steady-state mode	1.5 A
Picosecond pulse	25 nC
Pulse width	30 psec 4 to 100 nsec 0.25 to 10 μsec

National Synchrotron Light Source
Brookhaven National Laboratory
Upton, New York 11973

NATIONAL SYNCHROTRON LIGHT SOURCE

The National Synchrotron Light Source (NSLS) facility consists of a 750-MeV (9-electron bunch) storage ring for VUV and IR research and a 2.5-GeV (30-electron bunch) storage ring for X-ray research. Attractive features of the synchrotron radiation include high brightness and intensity, a broad and continuous spectral range, high polarization, and pulsed time structure (subnanosecond pulses). With each of the 28 X-ray and 16 VUV beam ports being further split into from 2 to 4 beam lines, it will be possible, when NSLS becomes fully operational, to have as many as 100 experiments running simultaneously. A 6-pole superconducting wiggler magnet and a 38-pole permanent magnet undulator have been constructed, and several wiggler and undulator magnets are presently being designed which will significantly increase the photon intensity and brightness.

The NSLS is a facility where a wide range of research techniques will be used by biologists, chemists, solid state physicists, metallurgists, and engineers for basic and applied studies. Among the techniques are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

USER MODE

The policy for experimental utilization of the NSLS is designed to enable the scientific community to cooperate in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines are being designed and instrumented by Participating Research Teams (PRT's). The PRT's are given priority for up to 75% of their beam line(s) operational time for a three-year term.

General Users will be able to perform experiments on an NSLS facility beam line or on a PRT beam line, which will be available for use by non-PRT members for at least 25% of its total operational time. For the PRT beam line, PRT's will provide liaison and utilization support to General Users. After an initial commissioning period, NSLS and PRT beam lines will become available for use by General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee will be charged for the amount of beam time utilized. The DOE has granted the NSLS a Class Waiver, under whose terms Proprietary Users of the NSLS will have the option to retain title to inventions that result from research performed at the NSLS.

A limited amount of funding will be available to scientists from U. S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky
NSLS, Bldg. 510E
Brookhaven National Laboratory
Upton, New York 11973

Phone:
Comm. (516) 282-4974
or FTS 666-4974

TECHNICAL DATA

Facilities	Key features	Operating characteristics
VUV electron storage ring	High brightness; continuous wavelength range ($\lambda > 5$ Å); 16 beam ports	0.75-GeV electron energy
X-ray electron storage ring	High brightness; continuous wavelength range ($\lambda > 0.5$ Å); 28 beam ports	2.5-GeV electron energy

Instruments	Key features
Monochromators	
Plane grating	12 Å $< \lambda <$ 1500 Å; high resolution
Zone plate	8 Å $< \lambda <$ 100 Å; moderate resolution
Toroidal grating	10 Å $< \lambda <$ 2500 Å; high intensity; moderate and high resolution
Extended range grasshopper	20 Å $< \lambda <$ 2000 Å; high resolution
Wadsworth	300 Å $< \lambda <$ 3000 Å; high intensity; moderate resolution
Seya and Czerny-Turner	1200 Å $< \lambda <$ 12000 Å; high intensity; moderate resolution
Two crystal	0.04 Å $< \lambda <$ 2500 Å; high resolution; fixed exit beam
Two crystal/two grating	2.5 Å $< \lambda <$ 2500 Å; high resolution; fixed exit beam
Six circle spectrometer/diffractometers	High positional and rotational accuracy
Experimental stations	Photoemission; magnetic circular dichroism; fluorescence; gas phase spectroscopy; microscopy; lithography; holography; EXAFS; inelastic scattering; crystallography; radiometry; topography; small angle scattering
Superconducting wiggler	$\lambda > 0.1$ Å; high intensity
Permanent magnet undulator	100 Å $< \lambda <$ 1000 Å; high intensity and brightness

Department of Physics
Kansas State University
Manhattan, Kansas 66506

JAMES R. MCDONALD LABORATORY

Three accelerators are operated primarily for atomic physics research. These accelerators are a 6-MV EN-tandem accelerator, a 3-MV Van de Graaff, and a 100-kV accelerator. Either foil or gas poststripping between the 90° and the switching magnet is possible for tandem beams. Available experimental facilities include (1) a 4.5-meter flight tube for impact parameter measurements, (2) curved crystal X-ray spectrometer, (3) spherical sector and cylindrical electron spectrometers, (4) hydrogen atom and metal vapor oven targets, (5) low-energy high-charge recoil ion sources, and (6) Si(Li), proportional counter, avalanche, and channel-plate detectors. The laboratory is available to users who require the unique facilities of the laboratory for experiments pertinent to DOE program goals.

COLLABORATIVE USE

Users are encouraged to seek a collaborator on the staff or can submit a brief proposal.

PERSON TO CONTACT FOR INFORMATION

Patrick Richard, Director
James R. McDonald Laboratory
Department of Physics
Kansas State University
Manhattan, Kansas 66506

Phone: (913) 532-6783

TECHNICAL DATA

EN Tandem

Beams: Most elements
Terminal voltages: 0.3 to 6 MV
Output currents: Up to 10 μA, depending on the ion species and the charge state
Repetition rate: DC or 3-nsec pulses at rates up to 4 MHz
Magnet limitations: $ME/q^2 \leq 150$

3-MV Van de Graaff

Beams: ^1H or ^4He
Terminal voltages: 0.3 to 3 MV
Output currents: Up to 100 μA
Repetition rate: DC only
Magnet limitations: None

100-kV Accelerator

Beams: Most elements
Terminal voltages: 20 to 100 kV
Output currents: Up to 10 μA, depending on the ion species
Magnet limitations: None

Notre Dame Radiation Laboratory
University of Notre Dame
Notre Dame, Indiana 46556

PULSE RADIOLYSIS FACILITY

The Notre Dame pulse radiolysis facility is based on a 5-nsec electron pulse from an 8-MeV linear accelerator. It is fully instrumented for computerized acquisition of optical and conductivity information on radiation chemical intermediates having lifetimes of 10 nsec and longer. Detectors having response times of ~2 nsec are available. For typical optical absorption studies, where one produces $10^{-5}M$ of intermediates, spectral and kinetic information can be obtained on species having extinction coefficients in excess of 100 $M^{-1}cm^{-1}$. Conductometric methods in aqueous solution cover the pH range of 3 to 11. Data are recorded digitally and stored in magnetically readable form for rapid off-line examination of spectral and kinetic details.

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists or by a proposal to the laboratory director.

PERSON TO CONTACT FOR INFORMATION

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Notre Dame Radiation Laboratory
Notre Dame, Indiana 46556

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TECHNICAL DATA

Electron source	8-MeV linear accelerator
Operating mode	Single pulse, with signal averaging
Data collection	PDP-8
Pulse width	5, 10, 20, 50 nsec
Time resolution (RC)	2 nsec
Pulse current	Up to 1 A
Repetition frequency	0.2 sec^{-1}

Optical absorption measurements	
Spectral region	210 to 750 nm
Sensitivity	±0.00002 absorbance
Conductivity	
pH range	3 to 11
Sensitivity	±5 mhos/cm

Operations Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

ELECTROMAGNETIC ISOTOPE SEPARATIONS (CALUTRON) FACILITY

The objective of this facility is to separate and provide multigram quantities of highly enriched separated stable and selected radioactive isotopes, including the actinides, to the research community. An important aspect of the program is the research, development, and demonstration of cost-effective alternate methods of isotope enrichment as well as activities in ion source technology, beam dynamics, ion retention, and chemical recovery procedures. All isotopically enriched samples are distributed through a regular sales program or are circulated to the research community on a loan basis from the Research Materials Collection, administered under the direction of DOE. The program is responsible for the production, distribution, quality control, and reprocessing of the material in the Research Materials Collection. Applications for the loan of samples from this collection for nondestructive research projects germane to DOE programmatic interests are received at any time.

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Physics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

EN-TANDEM

The EN-Tandem is operated primarily as an atomic physics facility. The highest terminal voltage is 6.5 MV. The widest possible variety of ion species are available from a selection of ion sources. Two 90° magnets with a stripper (gas or foil) between them follow the accelerator so that a range of charge states is available for any ion at a given energy. Available facilities include (1) a merged electron-heavy ion beam apparatus with a merged region ~1 meter in length; (2) an ~14-meter flight tube with the capability of doing very small angle scattering and detecting individual charge states; (3) a Penning ion trap apparatus; (4) an Elbeck magnetic spectrograph with position sensitive detectors; (5) Si(Li) detectors and a curved crystal spectrometer; (6) both low- (eV to keV) and high- (MeV) monoenergetic position sources (being developed).

COLLABORATIVE USE

Collaborative experiments may be arranged with appropriate staff scientists or by a research proposal to the EN-Tandem manager.

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TECHNICAL DATA

Beams: Most elements
Terminal voltages: 0.3 to 6.5 MV
Source beam currents: Several hundred nA to several μA
Output currents: Up to 1 μA, depending on the ion species and charge state
Repetition rate: DC only (at present)
Magnet limitations: $ME/q^2 \leqslant 80$

Operations Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

HIGH FLUX ISOTOPE REACTOR

The prime purpose of the High Flux Isotope Reactor (HFIR) is to make research quantities of ^{252}Cf and other transuranium isotopes. These materials are produced in the flux trap in the center of the HFIR fuel element where a thermal-neutron flux of 3×10^{15} neutrons/(cm^2 · sec) is available to irradiate the curium target material. The HFIR is a beryllium-reflected light-water-cooled and -moderated, flux-trap reactor with a design power level of 100 MW. It burns 93% enriched ^{235}U fuel in aluminum-clad plates. Additional irradiation facilities are provided in the beryllium reflector around the fuel element to increase the production rate of the heavy isotopes.

The HFIR also has, as a secondary purpose, the performance of diverse irradiations, tests, and experiments which benefit from the exceptionally high neutron flux available. In the fuel element flux trap, a hydraulic-rabbit tube provides access to the maximum thermal-neutron flux in the reactor for short-term irradiations, and other positions are ideal for fast-neutron irradiation-damage studies. The beryllium reflector contains numerous experiment facilities with thermal-neutron fluxes up to 1×10^{15} neutrons/(cm^2 · sec). These facilities can accommodate static experimental capsules, complex fuel-testing engineering loops, and special experimental isotope irradiations, the targets for which are prepared by the Oak Ridge National Laboratory Isotopes Group. Four beam tubes are used for neutron-diffraction experiments and a small-angle neutron scattering facility sponsored by the National Science Foundation is available for use by researchers from universities, industry, and other national laboratories.

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TRANSURANIUM PROCESSING PLANT

The objective of this program is to supply transplutonium elements for use in research. This involves operation of the Transuranium Processing Plant (TRU), which is the production, storage, and distribution center for the DOE heavy-element research program. Target rods are fabricated at TRU, irradiated in the High Flux Isotope Reactor (HFIR), and processed at TRU for separation, recovery, and purification of the heavy actinides up through ^{257}Fm. Since their construction in the mid-1960's, TRU and HFIR have provided the western world's supply of elements beyond curium (atomic number 96), either directly or by furnishing starting materials for further nuclear-synthesis reactions. The transuranium element isotopes produced in TRU are used nationally and internationally to study the basic physics and chemistry of the transuranium elements and, also, they are being used in research and development programs relating to environmental effects, biological effects, and waste isolation.

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Combustion Sciences Directorate
Sandia National Laboratories, Livermore
Livermore, California 94550

COMBUSTION RESEARCH FACILITY

Current activities at the Combustion Research Facility (CRF) supported by the Division of Chemical Sciences emphasize the development and the applications of new diagnostic techniques to the study of basic flame processes, as well as research in fundamental chemistry important in combustion. (These programs are individually described elsewhere in this publication). In addition, DOE/Conservation sponsors programs at the CRF in combustion technologies, and DOE/Fossil supports programs in coal combustion and related diagnostics development.

Complete facilities for resident and visiting researchers are available: offices for 60 staff, a meeting room accommodating 250 people, a laboratory building housing 14 independent experiments, special facility laser systems, a dedicated VAX computer, and access to a Cray computer.

The facility is located in Livermore, California, in the San Francisco Bay area, near major universities and other U. S. Government supported laboratories.

USER MODE

Qualified scientists are encouraged to take advantage of the specialized resources available at CRF. Prospective participants should submit a brief proposal to the laboratory director. Criteria for selection include technical merit, the extent to which CRF facilities are used, overlap with DOE program objectives, and the availability of specific equipment.

In general, the CRF will host visiting scientists to use the special-purpose lasers, work with resident staff, make use of computers and codes, and set up experiments. Visitors pay for their own salary, travel, housing, meals, and other local expenses. Facility lasers, apparatus, technicians, instrumentation, computers, and support-group services are provided without charge for research that is not proprietary. Research results from nonproprietary projects are expected to be published and disseminated.

For scientists with active government contracts, support for CRF research often can be arranged on an informal basis with the contract manager. There are opportunities for faculty, postdoctoral scientists, and graduate students to obtain Sandia support for combustion-related research at CRF.

In specific instances, proprietary research can be carried out at CRF. For this type of work, the DOE will be reimbursed on a full cost recovery basis for the use of all CRF resources. Details of a DOE Class Waiver for patent rights are available.

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or	
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TECHNICAL DATA

Equipment	Key features
Flashlamp-pumped, tunable dye laser	Long pulse, high energy, high average power: 2-μsec pulse length 5 J/pulse, 10 Hz Tunable 440 to 620 nm 0.03-nm bandwidth
Multipurpose pulsed laser system	High peak power, high resolution doubled YAG and tunable dye lasers: Single mode capability 10 to 500 mJ/pulse 10 to 20 nsec/pulse
Low-pressure flames	10 μ to 1 atm Mass spectrometer sampling probe
Atmospheric flames	Diffusion and premixed flames
High-pressure flame	Combination of diffusion flame burner with high pressure flow chamber: Pressures up to 20 atm Slot-geometry burner 2-0 laminar diffusion
Vertical turbulent diffusion flame	Open-circuit, induced-draft wind tunnel with co-flowing axisymmetric fuel jet: 30- by 180-cm viewing section to 6000 scfm flow
Atmospheric Combustion Exhaust Simulator (ACES)	Atmospheric pressure combustion exhaust chamber: To 1200°C 0.5 to 100 m/sec flow speed Trace species and particulates Optical and physical probes Materials test section

Equipment	Key features
Combustion bomb	Simulates constant-volume engine combustion
Internal combustion research engines	Highly repeatable environment for homogeneous charge and diesel combustion studies
Experimental diagnostics research facilities	Laser fluorescence laboratory
	Coherent Raman spectroscopy laboratories
	Laboratory for laser ionization, saturation, optogalvanic detection of trace species
	Kinetics laboratories with tunable quasi-cw UV and ring dye lasers for analysis; excimer lasers for photolysis
Computing facilities	Minicomputers in laboratories Access to CRF VAX 11/780 Access to Sandia National Laboratory, Livermore, CRAY via in-house staff

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Summaries of the FY 1984 and FY 1985 Applied Mathematical Sciences Research Program

July 1985

U.S. Department of Energy
Office of Energy Research
Scientific Computing Staff
Applied Mathematical Sciences
Washington, D.C. 20545

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PREFACE

The purpose of this report is to provide a convenient compilation of summaries of the individual research projects that constitute the Applied Mathematical Sciences research subprogram managed by the Director, Scientific Computing Staff, Office of the Director of Energy Research, Department of Energy. This new office, organized in 1984, consists of the applied mathematical sciences research activity formerly under the Division of Engineering, Mathematical and Geosciences, Office of Basic Energy Sciences, Office of Energy Research, and the management of the expanded National Magnetic Fusion Energy Computer Network formerly under the Office of Magnetic Fusion Energy. The organization chart on the next page illustrates the structure of the basic research arm of DOE - the Office of Energy Research. The personnel responsible for this subprogram are:

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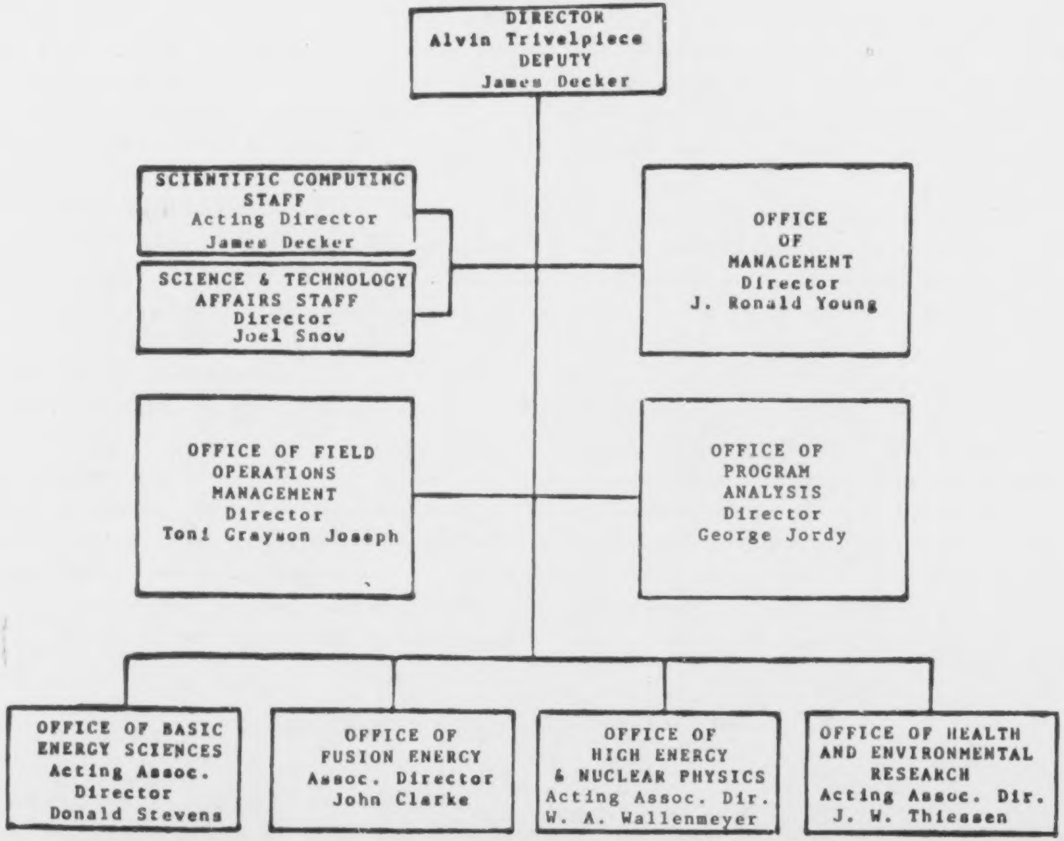
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Department of Energy
Office of Energy Research
Office of the Director
Scientific Computing Staff
Applied Mathematical Sciences Research Subprogram

Overview

The Applied Mathematical Sciences Research subprogram consists of two parts: Energy Science Advanced Computation and Applied Mathematical Sciences Supercomputing Research. The Energy Sciences Advanced Computation activity provides scientific supercomputer access required by researchers in the Office of Energy Research programs in High Energy and Nuclear Physics, Basic Energy Sciences, and Biological and Environmental Research. This scientific computing will be provided through network access to supercomputers for contractors in universities, industry, and DOE national laboratories. The Supercomputing Research activity supports research in mathematics and computer science that is essential to the use by many DOE programs of the newly emerging multiprocessor supercomputer systems and the long range development of future supercomputer systems. In addition to meeting DOE needs, this subprogram will make a substantial contribution to solving the national problems of providing access to researchers, particularly in universities, and maintaining U.S. leadership in supercomputer technology.

Supercomputers are the fastest general purpose scientific computers available to solve large scale scientific problems. They are today capable of performing 100's of millions of arithmetic operations per second and have several million words of fast memory. The effort in large scale scientific supercomputing is distinguished from the Japanese Fifth Generation project and DARPA's Strategic Computing and Survivability program, which are focused on artificial intelligence techniques.

In recent years, the modern supercomputer has changed the nature of scientific research and technology development. The advancement of science used to depend upon experiments for data and theory for understanding. Today there is a third equally important ingredient to scientific research: computational science. Computational science serves a role that is a hybrid between theory and experiment. In some cases, computations provide insights into experimental data, and in others, computations are used to simulate the ideal experiment to test an analytical model. The emergence of computational science is an important element in scientific research and technology development is the result of the development of our ability to do computational modeling of complex physical problems and the enormous power of the modern supercomputer. This combination allows scientists and engineers to model complex problems in a much more realistic way and to obtain much more accurate answers than was possible just five years ago.

Scientific supercomputing now makes substantial contributions to many fields of research such as fluid dynamics, plasma dynamics, astrophysics, materials science, chemistry, atomic physics, etc. Similarly, large scale calculations are making significant contributions to product development in areas such as nuclear weapons, electronics, automobiles, aircraft, and chemicals. In product development, computer modeling is used to reduce the number of design/test iterations which are so time consuming and expensive.

The Department of Energy has made a significant commitment to large scale scientific computing in several of its research and development programs. As an agency, DOE is the largest user of supercomputers in the world. In 1985 DOE laboratories will house 22 supercomputers. DOE's commitment to scientific computing is not new. Historically, the Department and its predecessor agencies (the Atomic Energy Commission and the Energy Research and Development Administration) caused many supercomputers to be developed through its nuclear weapons design work at the Lawrence Livermore National Laboratory and the Los Alamos National Laboratory. The supercomputers that were developed in response to DOE needs were delivered to the DOE laboratories nearly devoid of software, requiring our laboratories to develop the necessary software for a complete supercomputer system. Through the software development efforts and the continual interaction between DOE laboratories and the supercomputer vendors, DOE has made significant contributions to supercomputer technologies.

DOE's commitment to scientific supercomputing has paid large dividends. Typical use of supercomputers in the Department's mission oriented development programs is to supplement or replace expensive, time consuming experimental testing with computer simulations. The advantages of such simulations to replace some of the testing in the nuclear weapons development programs are obvious. In a research and development program such as magnetic fusion where experiments cost $10's to $100's millions and take 3-7 years to build, it is impossible to build a new device and test experimentally every good idea that comes along. Computer simulation has become essential.

Great progress has been made in our ability to do computer modeling of complex scientific problems; however, there is still a long way to go. Many of the Department's research and development programs have large, complex research and engineering problems to solve that can be only crudely approximated with today's supercomputers and mathematical techniques. There is a need to include more "physics" in the models, to use finer zoning for more accurate answers and to use more dimensions. In order to solve these complex problems to the accuracy desired in the future, computers with substantially increased computing power over those currently available will be required. Several DOE programs have estimated that they will require computers 200 times as powerful as a Cray-1 or a Cyber 205 by the end of the decade. In fact, some of the DOE programs could use that kind of computing power today, if it were available.

Interagency Coordination of Supercomputer Access and Research Programs

In 1983, the White House Office of Science and Technology Policy (OSTP) established three subcommittees under the Federal Coordinating Council on Science, Engineering, and Technology (FCCSET) to examine the U. S. role in maintaining leadership in the development and use of supercomputer technology. Membership on these subcommittees includes representatives from DOC, DOD (including DARPA, CIA, and NSA), DOE, NASA, NSF, and OSTP. The subcommittees were charged with developing recommendations on the role of the government in maintaining the U. S. lead in supercomputers, on providing access to supercomputers for our researchers, and on coordinating the roles of each agency in the area of research on artificial intelligence and high performance computing. Each of these subcommittees produced reports for OSTP and continues to provide coordination among agencies in these areas.

Two of the subcommittees, one addressing government supercomputer procurement policies and the other addressing access to supercomputers for researchers, were combined into a single subcommittee, chaired by Dr. James Decker, DOE. This subcommittee maintains contact with industry representatives, sponsors panels to investigate questions concerning computer network access to supercomputers and interagency sharing of resources.

The third FCCSET subcommittee is chaired by Dr. Robert Kahn, DARPA, and its charter is to stimulate the exchange of information within the government on high performance symbolic computing and artificial intelligence. During the course of its initial deliberations it became clear that interest in information exchange extended beyond symbolic processing and AI. It was decided to broaden the charter of this subcommittee to include federal research efforts in very high performance scientific and numerical computing and advanced computer research. A report, entitled "Report of the Federal Coordinating Council on Science, Engineering, and Technology Panel on Advanced Computer Research in the Federal Government," June 1985, has been submitted to OSTP.

Another interagency group that has been coordinating research for many years is the Interagency Committee on Extramural Mathematics Programs (ICEMAP). Active members of this committee include representatives from DOE, DOD (AFOSR, ARO, and ONR), and NSF. Occasional participation in the ICEMAP activities include representatives from NIH, NASA, CIA, NSA, and DOC (NBS). In FY 1985, the ICEMAP agencies cooperated in establishing the Board on Mathematical Sciences in the Commission on Physical and Mathematical Sciences of the National Research Council in the National Academy of Sciences.

Energy Sciences Advanced Computation

The Energy Sciences Advanced Computation activity provides OER research access to supercomputers over nationwide networks, including the NMFECC satellite network, the ARPANET, and commercial value-added networks. Although DOE has been a leader in the use of supercomputers in its defense and magnetic fusion programs, there are several research programs that have not had easy access to modern supercomputers. In FY 1985 the use of the National Magnetic Fusion Energy Network was expanded to researchers supported by the Department's High Energy and Nuclear Physics, Basic Energy Sciences, and Biological and Environmental Research programs. A Cray-XMP/22 was added to the computer capacity at the MFE center at Livermore and expansion of the communications network was begun. In addition, a new supercomputer research institute at Florida State University was initiated at the direction of Congress. A Cyber 205 supercomputer at FSU was installed and linked to the MFE network in early 1985 for use by OER researchers. This activity is described in DOE Report Number DOE/ER-0218, "The Role of Supercomputers in Energy Research Programs," February 1985.

The Research Activity

The primary objective of the research activity is to advance the understanding of the fundamental concepts of mathematics, statistics, and computer science underlying the complex mathematical models of the key physical processes encountered in the Department's research and development programs. In addition, this activity supports investigations of parallel computer architectures that may lead to new approaches to supercomputers. The Supercomputer Research activity provides the primary source of research funding for applied mathematics and computer science research to meet the DOE needs in this area.

One of the primary goals of this activity is to develop our ability to use multiprocessor computer systems. The multiprocessor direction for supercomputers is dictated by the fact that only very limited gains can be made from increased component speeds and levels of integration in the future. This has caused computer architects to look to using more than a single processor working on a problem. In the near term, the supercomputer vendors are producing systems with 2-16 processors. In the longer term, systems with 100's to 1000's of processors are expected.

The change from von Neumann (sequential) to parallel processor machines represents an enormous change in scientific computing, greater than the challenge faced by the introduction of vector processors. The challenge with parallel processors is to have a large number of processors efficiently working simultaneously on the same problem. New software, languages, algorithms, and even entirely new mathematical approaches to solving important classes of scientific problems be will required. One of the objectives of this activity is supporting research on parallel computing necessary to ensure that the Department's programs requiring scientific supercomputing will have the tools to use efficiently the new machines as they become available and to exploit their maximum capability.

The DOE scientific research community comprises a large fraction of this nation's expertise in large scale computational modeling, with applications in fusion energy, weapons design, and fundamental physical sciences research. Much of the scientific research and development effort throughout DOE programs is focused directly on analytical and numerical modeling of physical processes. An understanding of the fundamental principles upon which these models are based is important for developing energy systems for the future. Thus, research in mathematical analysis, algorithms, and computational techniques forms the knowledge base for conducting scientific research. DOE's lead role in the development and application of supercomputing techniques is based on this fundamental research.

The subprogram funds basic research at many of the national laboratories, universities, and private research institutions in three major activities: Analytical and Numerical Methods, Information Analysis Techniques, and Advanced Computing Concepts. In addition, experimental computing capabilities were established as research facilities to support the exploration of new concepts in large scale scientific computing. Regular meetings with program managers in other Federal agencies help coordinate these activities.

In FY 1985, an enhancement in the research effort in large scale scientific computing was started, with emphasis on algorithms for large scale parallel architectures based on several experimental computer systems under study. The emphasis on new parallel multiprocessor architectures applies to all three activities of the research activity: analytical and numerical methods for the solution of systems of differential equations, information analysis techniques, and advanced computing concepts.

This activity will greatly accelerate the pace of projects in parallel supercomputing so that some of the research machines can be brought to a usable state as soon as possible. Also included in the long range plan for this activity is an expanded participation by interdisciplinary teams working on problem decomposition, algorithm development, numerical analysis, performance evaluation, and languages for highly parallel architectures.

The R&D projects supported by this activity have two important facets requiring substantial cooperation and coordination among traditionally separate groups. One facet is interdisciplinary teams of computational scientists, computer scientists, and mathematicians working on all aspects of large scale scientific computing problems. The other is the cooperation of industry, government and universities on the design and implementation of prototypes of several potentially strong candidate architectures; this will be an important proof of concept activity.

The university researchers play the major role in generating ideas and research software and in training graduate students in generating new applications. National laboratory staff are in the forefront of tackling real world, large scale scientific problems and have unique resources for participating in these research projects. Industry likewise has a unique role in providing state of the art production and testing facilities and stands to reap great benefits in understanding future architecture and software issues that tend to limit industry use of supercomputers currently. The transfer of technology from the academic and laboratory research environment to industry could be as rapid as possible through these cooperative projects. The DOE program will be coordinated with the other agencies to share common facilities where possible, such as very large scale integration (VLSI) design facilities and component fabrication.

Analytical and Numerical Methods

This activity supports the investigations of the fundamental properties of mathematical models used to simulate complex physical phenomena observed in energy systems. This category includes applied analysis, numerical methods for solving large systems of differential equations, and numerical analysis of algorithms.

These funds support interdisciplinary teams including analysts, applied mathematicians, computational scientists, postdoctoral fellowships and graduate students collaborating in universities and national laboratories to research parallel algorithms for mathematical software tools used in implementing these models. As documented in the David Committee's report, "Renewing U. S. Mathematics: Critical Resource for the Future," published by the National Research Council of the National Academy of Sciences, DOE's research program in applied mathematical sciences plays a lead role in support of basic research at the interface between mathematical and computational sciences. The shortage of graduate students and post-doctoral support in this crucial area is becoming severe and the current demand for trained computational scientists by industry is rapidly draining the academic pool and the pool of talent available to the National Laboratories. The intent is to strengthen the ties between universities and the Labs and to provide salary support and computational resources in the disciplines associated with computational science. The DOE program, with its unique history of basic research in these areas, is positioned to provide strong leadership in filling the "pipeline" from graduate studies to postgraduate studies to research positions in academia and the Labs.

Information Analysis Techniques

This activity supports the investigation of data management and statistical analysis of large scientific data sets common in DOE mission programs, such as High Energy Physics, Magnetic and Inertial Fusion, and others. Funding here supports advanced work in computational statistical methods and in techniques for managing the large scale scientific databases common to many DOE mission applications. The existence of a large set of valuable scientific databases in the DOE multiprogram and single purpose laboratories provides a unique resource for basic research in this area. Very few universities have the opportunity to study real scientific databases of the complexity found in our mission programs; a strong research effort in this area must be supported if huge data management and analysis problems are to be solved.

Advanced Computing Concepts

This activity meets a wide range of problems associated with the effective use of large scale scientific computers for the

Department's research and development program. The areas of research include software engineering techniques for design of quality mathematical software, distributed systems, and parallel architectures for high performance scientific computers. A variety of new techniques for decomposing large problems to execute on a large number of concurrent processors is being investigated in DOE laboratories and universities. These techniques will provide the insight needed to build the supercomputers of the 1990's.

These new architectures, employing perhaps hundreds or thousands of fast processors working concurrently to solve a single problem, require a thorough reexamination of all aspects of the solution method. Problems must be decomposed into parallel steps for concurrent execution. Algorithm characteristics such as accuracy, stability, robustness, and correctness of implementation must be investigated anew.

This activity supports joint university/industry/laboratory projects for the design phase of research parallel architectures started in FY 1985. Several projects have been supported over the past few years to design, analyze and simulate a variety of innovative multiprocessor architectures. Typically, these projects have been supported at the level of $100,000 to $500,000 per year to demonstrate the feasibility of implementing large scale computational models common in DOE programs. These projects are now expanding to the implementation phase to demonstrate and evaluate the capabilities of these architectures for future supercomputers. In FY 1985, several projects were supported at the level of between $1,000,000 and $2,500,000 per year to provide for implementation and software development of research machines. Each project represents a collaboration among universities, national laboratories, and private industry.

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
** Budget and Reporting Activity: KC 070101							
Ames Laboratory, Iowa State University	James Corones/	Analytical and Numerical Methods - Wave Propagation	The Applied Mathematical Sciences program at Ames is exclusively in the area of applied analysis. This effort is focused on basic and applied problems of wave propagation. Particular attention is given to direct and inverse scattering theory and their applications. The purpose of this work is to develop mathematical procedures and tools that can be used to characterize and/or image nonuniformities in materials (density variations, stress fields, cracks, potential variations, for example). Two types of approaches are employed: 1) direct scattering, in which the nonuniformities are given and the objective is to compute the scattered field (e. g., of elastic waves scattered by cracks) and thereby determine characteristic signatures of scatterers; and 2) inversion procedures, in which incoming and outgoing signals are assumed known and the objective is to deduce the characteristics of the nonuniformities from this knowledge. Our inversion studies incorporate realistic constraints such as limited angle softview, limited apertures and noise. The techniques developed have wide application, including quantitative NDE (QNDE), geoprospecting, remote sensing of nuclear waste, plasma diagnostics, and fission reactor diagnostics. At present, QNDE is the major applications orientation of the effort. In addition, there is work on special functions directed at facilitating their use and computation.	10/01/85	09/30/86	400	475

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Argonne National Laboratory	Paul Messina/ Hans Kaper	Analytical and Numerical Methods	Applied analysis research involves the application of analytical and numerical techniques to problems in the natural and engineering sciences. Major efforts focus on spectral analysis of differential operators and bifurcation and stability analysis of nonlinear phenomena in combustion. In addition, research continues on modeling and analysis of certain fluid flow and materials science problems. Computational mathematics research involves the design and analysis of numerical algorithms, the development of special techniques to measure algorithm reliability and efficiency, and the preparation of software based on broadly portable algorithms for vector and parallel computers. New studies have also begun on defect migration phenomena, high dimensional quadrature, optimization techniques for Stirling engine design, and evaluation criteria for parallel algorithms. Use of our advanced computing research facility, as well as advanced computer systems at other sites, is essential for this investigation.	10/01/85	09/30/86	950	950
Atlanta University	Ronald Mickens/	Investigation of Perturbation Techniques for Nonlinear Difference Equations	Our major research activity will be the construction of a number of regular and singular perturbation techniques which may be used to obtain approximate analytical solutions to several classes of nonlinear difference equations. We will put particular emphasis on those procedures that lead to uniformly valid asymptotic solutions. An investigation will also be carried out on the modeling of nonlinear, first order ordinary differential equations by difference equations. In particular, procedures that give rise to models with zero local truncation error will be emphasized.	08/01/83	07/31/86	67	83

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Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Brookhaven National Laboratory	Ronald Peierls/ Robert Marr	Analytical and Numerical Methods	This task involves the application of analytical and numerical techniques to investigate and develop computational methods for problems that arise in a variety of scientific and engineering contexts of importance to DOE. The goal is to develop methods that are both reliable and efficient. Much of the current emphasis is on more realistic modeling of three dimensional problems and towards the understanding of nonlinear effects. Even the most efficient methods imply massive computational requirements which will only be met by computers with parallel architectures. Specific areas of research include the numerical modeling and solution of direct and inverse wave propagation problems; the discretization of linear and nonlinear elliptic boundary value problems using finite element and finite difference methods; and the application of iterative solution methods such as preconditioned conjugate gradient methods to the resulting systems of equations. In image reconstruction, development of algorithms for nuclear magnetic resonance imaging continues. with current emphasis being on the use of projection reconstruction methods for spatially imaging chemical shifts, the investigation of filtered back transform reconstruction algorithms and inherent performance characteristics of generalized Fourier methods, and the investigation of a new imaging strategy based on stochastic NMR techniques.	10/01/85	09/30/86	457	360

Summary of Applied Mathematical Sciences Research Projects
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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
California Institute of Technology	Herbert Keller/ Philip Saffman	Numerical Analysis, Computing and Fundamental Studies of Energy...	The work is concentrated in two main areas: hydrodynamics and numerical methods for the solution of partial differential equations. The hydrodynamics work includes vortex dynamics, turbulent flow, shear flow, and flow in porous media. The main emphasis on numerical methods development has been in the general area of path following and continuation methods, including global Newton and homotopy methods. These methods have been used along with finite difference and spectral methods for solving two point boundary value problems, partial differential equations and integral equations. Adaptive mesh selection and curvilinear overlapping grid methods are beginning to be used. Additional effort will be aimed toward the development of software for accessing remote large scale scientific computing resources.	04/01/83	03/31/86	259	271
Columbia University	Michael Tabor/	Singularity Structure of Nonlinear Ordinary and Partial Differential Equations	This project aims to study both nonlinear ordinary and partial differential equations from the point of view of their singularity structure. For ordinary differential equations the property that the solutions be meromorphic (in time) seems to provide a test of integrability for these systems. Our aim is to provide an in depth understanding of this technique and to extend its range of applicability. In the case of partial differential equations a similar concept has been developed involving the theory of functions of many complex variables. The validity of this technique, its extensions and its relationship to other methods in the field of integrable systems are to be investigated in detail. Overall, the program aims to provide a unified approach to a wide variety of nonlinear equations and the many physical processes that they model.	05/01/84	04/30/87	57	63

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Cornell University	Thomas Coleman/	Topics in Large Sparse Nonlinear Optimization	Many problems in the physical science, engineering, and econometric disciplines involve the numerical solution to a system of nonlinear equations or the computation of the minimizer of a nonlinear function. Often these nonlinear problems are of large dimension involving several hundred to several thousand variables. Typically, the relevant Jacobian and Hessian matrices are sparse. In addition, it is often the case that a single evaluation of the function or gradient is an expensive operation. The purpose of the proposed research is to explore ways in which sparsity can be exploited so that the number of function (or gradient) evaluations is 'minimized' and yet a solution is efficiently obtained. In particular, this project will examine several computational questions concerning the efficient estimation of a sparse symmetric Jacobian matrix by finite differences and the economic use of partial Jacobian information. Also, this research will examine several related issues that arise when minimizing a large sparse nonlinear function in the presence of constraint functions.	05/01/83	04/30/86	44	52
Cornell University	Mitch Feigenbaum/ Eric Siggia	Systems Near the Onset and in the Well Developed Regimes of Turbulence	We present a program of research dedicated to chaotic behavior in both the onset regime and in the fully developed (or high modal) regime. The investigations proposed entail a blend of a computational effort to gain data supporting the insights, and assisting the development, of a theoretical effort employing recently developed methodologies and ideas. The first aspect of this program - work pertaining to the onset of turbulence - is founded on the fact that universal minimal (and low) modal models can successfully embrace the behavior of real continuum systems. Our attack includes the investigation of chaos borne from low order quasiperiodicity; modifications of these phenomena in the presense of spatial symmetries; the continued investigation of functional integrals in order to determine the sensitivity of these processes to external noise and an attempt to develop descriptions of the fractional dimensional attractors that determine post onset turbulence. The second aspect of our research is centered on intrinsically high modal turbulence arising either from the onset behavior in large cells or from high Reynolds' number excitations. In the first case, we intend to continue investigations of theories to describe pre-Hopf bifurcation drifts in degenerate spatial structures. In the case of fully developed turbulence, we intend to perform investigations of details of the flow that can clarify the role of large scales in determining small scale intermittency.	01/01/83	12/31/85	171	187

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Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Cornell University	Geoffrey Ludford/	Special Year 1984-1985 on Reacting Flows: Combustion and Chemical Reactors	The Center for Applied Mathematics at Cornell will conduct a year long research meeting on reacting flows (combustion and chemical reactors). The Special Year will consist of eight distinguished speakers brought in during the academic year, culminating in the two week AMS-SIAM Summer Seminar, which was awarded to Cornell for this purpose. The object is to synthesize the newly emerged theory of reacting flows up to its interface with the computation of such flows and to preserve the knowledge gained from this activity in a Proceedings volume that will provide a firm foundation for future research in the computational aspects of reacting flows. (Note: This Special Year was jointly funded by Applied Mathematical Sciences, Engineering Sciences, and Chemical Sciences.)	09/01/84	08/31/85	23	0
Indiana University	Cyprian Foias/	Criteria for the Reliability of Numerical Approximations to Fluid Flow Problem	The numerical approximation of the solutions of fluid flow models is a difficult problem encountered in many areas of energy research. In all numerical methods implementable on digital computers, the basic question is how to choose the number of elements, N say (Galerkin modes, finite difference cells, finite elements, etc.) in order to guarantee that the approximation at least behaves like the exact solution. In the absence of a rational prescription for the determination of this number until now, it has been estimated either empirically or on the basis of physical intuition. The purpose of this research is to derive useful estimates for N from some newly discovered fundamental properties of the viscous incompressible Navier Stokes equations.	05/01/82	08/31/85	72	0

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Kent State University	Richard Varga/ Paul Wang	Applications of Numerical Analysis and Computer Symbolic Computation	The emphasis of this research is on the theoretical basis for workable numerical algorithms for general iterative methods in linear algebra and for coupling of the construction of these algorithms with symbolic algebra systems. Three areas are under investigation: (1) An asymptotic analysis of basic iterative methods for solving matrix equations arising primarily from the use of finite element methods; (2) The use of symbolic and numerical techniques to attempt to settle longstanding conjectures in function theory and in approximation theory; and (3) The integration of symbolic and numerical computing techniques.	12/01/83	11/30/86	103	108
Lawrence Berkeley Laboratory	Paul Concus/ Alexandre Chorin	Analytical and Numerical Methods	The analytical and numerical methods program at LBL focuses on the development of techniques for use in mathematics, physics, and engineering. Common to the various projects is the design of new methods that utilize computer resources effectively to provide fast and efficient algorithms, with the goal of illuminating increasingly complex and realistic physical and engineering phenomena. The physical topics include fluid dynamics, high speed gas flow, turbulence theory, the dynamics of fronts and interfaces, combustion, capillarity, and image reconstruction. The techniques developed and used include vortex methods, high resolution methods for hyperbolic equations, fast enumeration methods, numerical integration in function spaces, and iterative methods for algebraic systems.	10/01/85	09/30/86	645	600

Summary of Applied Mathematical Sciences Research Projects
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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Lawrence Livermore National Laboratory	Robert Huddleston/ James McGraw	Computational Mathematics	Computational mathematics research focuses on the design, development, and testing of algorithms to solve problems more accurately and/or more efficiently than existing methods, and to solve problems that have been intractable using existing algorithms. Research on adaptive methods for solving PDEs on multiprocessors will be expanded to include local grid refinement methods. Research on adaptive methods involving moving grids will continue. In addition, research will continue on the multiprocessor solution of algebraic systems arising from an implicit time step on a large stiff system of ODEs, and on shape preserving and scattered data interpolation and approximation methods for bivariate functions. In all of these areas attention will be focused on algorithm development and implementation on multiprocessors.	10/01/85	09/30/86	175	250
Los Alamos National Laboratory	George Bell/ Basil Nichols	Numerical Algorithms and Nonlinear Mathematics of Energy Systems	In adaptive numerical methods, we are constructing both static and dynamic reasoning algorithms; we are addressing the concept of dynamic processor allocation strategy for their implementation on machines with advanced computer architectures. Other developments include: composite grids; interface tracking through adjustment of the new grid on the moving boundary; high order collocation methods and supra-convergent difference schemes on irregular grids; semi-coarsening in multigrid methods and blackbox multigrid software. We are concurrently developing and demonstrating the concept of adaptive mesh refinement using the multigrid method; our testbed is an existing highly vectorized 3-D Eulerian multigrid finite element code. We are investigating 3-D front tracking methods as to their compatibility with the multigrid framework. We expect the implementation of the multigrid framework to be highly effective on machines with massively parallel architectures. Jointly with the Center for Nonlinear Studies at Los Alamos, the main thrust of our effort in applied analysis is directed at investigating pattern selections, instabilities, and chaos on strongly dissipative interfaces in flows. For this class, we establish genuine low modal behavior and we construct explicit formulas for the low fractal dimension of the strange attractor as a function of a typical pattern size, in the post onset turbulence regime. We demonstrate that these PDE's are rigorously equivalent to a low dimensional dynamical system; we establish the existence of a universally attracting, compact, finite dimensional inertial manifold. Future efforts are aimed at further bridging the gap between dynamical systems and PDE's.	10/01/85	09/30/86	325	350

Summary of Applied Mathematical Sciences Research Projects
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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
New York University, Courant Institute	Peter D. Lax/ James Glimm	Analytical and Numerical Methods	Two remarkable developments have taken place in many of the high technologies: the replacement of much experimentation by computer simulation, and the digital storing and processing of information. The reason for the former is the enormous gain in economy and flexibility of computer simulation over experimentation. This is particularly true in the energy related technologies; it is worth pointing out that the AEC was among the first of the technologically oriented organizations to recognize that in order to carry out its mission, it had to rely on a tremendous amount of computer modeling. A very large percentage of the relevant models are described in terms of partial differential equations. The success of solving these equations depends critically on the availability of new computing methods and efficient algorithms for implementing them. This is borne out by a glance at the history of scientific computing; it shows that each advance was at least partly fueled by an improved numerical method. As examples of such ideas, one can point to shock capturing, alternating direction, high order difference methods, finite elements, use of complex coordinates, random choice, discrete vorticity, spectral methods, implicit methods, flux corrected transport, adapted mesh, and others. In the last five years this Laboratory has been active in the design of a novel highly parallel computer. In the next two years we expect to devote a significant portion of our effort to devising algorithms suitable for such an architecture. The Courant Institute was always deeply involved in the invention and development of methods for solving partial differential equation, and this pursuit continues to be a significant portion of the scientific program of the Courant Mathematics and Computing Laboratory.	10/01/85	09/30/86	1210	1162

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Northwestern University	Bernard Matkowsky/	Research in Nonlinear Problems of Energy	Faculty associates on this project are Profs. M. Matalon, T. Erneux, Z. Schuss, and A. van Harten. A concerted attack on a large variety of problems involving the transition from laminar to turbulent combustion will be made. The program will involve several faculty members and research associates including postdoctoral students. The program is a theoretical effort, closely coordinated with experimental work. In this program, several relevant problems that are governed by systems of nonlinear ordinary and partial differential equations will be studied. Specific problems under investigation are: application of the Matalon-Matkowsky model of flames with nonzero thickness to the stability of curved flames; secondary bifurcation from cellular or pulsating flames; downward flame propagation in long vertical channels; burner stabilized flames in more than one dimension; interaction of flames with sound; and application of stochastic differential equations to the problem of relative stability of various multiple stable states of a system, including the derivation of more accurate expressions for chemical reaction rates.	01/01/84	12/31/87	100	105

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Oak Ridge National Laboratory	Robert Ward/ Michael Heath	Computational Mathematics	Research in computational mathematics is concentrated in numerical linear algebra, with the focus on problems involving sparse matrices in the areas of systems of linear equations, eigenvalue problems, and least squares approximations. Our current emphasis is on development of both general methodology and specific algorithms for matrix computations on parallel computers. In two separate, but related, lines of research we are developing both data flow and control flow algorithms for parallel computation of the Cholesky factorization. This work will be extended to include both symbolic and numeric phases of sparse factorization. We are also developing a block Jacobi algorithm for symmetric eigenvalue problems for parallel computation using systolic arrays. Our work on the M matrices arising from queuing networks and Markov chains will continue, including the analysis of both direct and iterative methods for solving homogeneous linear systems involving such matrices, as well as updating sensitivity analysis, and iterative refinement.	10/01/85	09/30/86	210	290
Oak Ridge National Laboratory	Robert Ward/ Allan Solomon	Applied Analysis	Research in applied analysis is carried out in two problem areas: moving boundary problems and stochastic analysis, with primary emphasis on the first topic. Work in moving boundary problems concerns the analysis of heat and mass transfer processes involving a change of phase. The mathematical questions are those associated with properly posing and analyzing, both qualitatively and quantitatively, the partial differential equations used to represent the idealized process. Our attention has been focused on modeling binary alloy solidification, with emphasis on the study of "mushy" zones and the initial behavior of phase fronts. This work will be complemented with new studies, such as hyperbolic heat transfer. Work in stochastic analysis concerns the modeling of disordered systems such as liquids and amorphous solids. Here the mathematical questions are associated with the spectral properties of certain operators which give information from the mathematical models of specific systems. This work has also become involved with alloy solidification, but with nonequilibrium or "ultrafast" solidification resulting in amorphous alloys.	10/01/85	09/30/86	205	210

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Rice University	Richard Tapia/ John Dennis	Quasi-Newton Methods for Unconstrained and Constrained Optimization	Researchers associated with this contract include Trond Steihaug of Rice University and Homer Walker of the University of Houston and their graduate students. The objective of this work is to extend the theory of quasi-Newton methods for unconstrained and constrained optimization. In the area of unconstrained optimization we have produced some theory that covers the situation when the objective function is known to possess noise and cannot be accurately evaluated. In constrained optimization we have developed a general convergence theory and have derived several new algorithms.	08/01/82	12/31/85	0	84
Sandia National Laboratories, Albuquerque	Lawrence Shampine/	Mathematical Software	Fundamental research in the numerical solution of ODEs leading to improved understanding of the task and to more efficient and reliable mathematical software: New understanding and improved estimates of local errors will be achieved. Several kinds of standard methods will be made more efficient and reliable. Global (true) error estimates will be devised. New methods for the solution of stiff problems will be proposed. A comprehensive package of Bessel functions of complex argument and nonnegative orders will be constructed. For maximum applicability and efficiency, each code requires the use of many methods. This necessitates fundamental mathematical and software research as well as extremely careful development and testing. Mathematical tools for solving inverse problems involving systems of ODEs will be developed. These tools will include better methods for solving constrained optimization problems and more efficient methods for solving systems of ODEs. Resulting codes will be used in the development of software for solving chemical kinetics parameter estimation problems and seismic parameter estimation problems.	10/01/85	09/30/85	210	225

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Sandia National Laboratories, Livermore	Robert Kee/ Linda Petzold	Analytical and Numerical Methods	This research is concerned with the solution of disparate scale partial differential equations; the approach is both analytical and computational. Although the results of this work are applied generally, one unifying theme is the interest in the problems that arise in combustion modeling. On the analytical side we are developing asymptotic models that explain instabilities in flames, alloying reactions, and solid propellants. On the computational side, we concentrate on large systems of stiff PDE's, particularly those that occur in models involving systems of complex chemical reactions. To achieve accuracy and efficiency in time dependent problems we are developing implicit methods, such as backwards differentiation formulas and implicit Runge Kutta, that deal effectively with the widely varying time scales that are present in chemical kinetics models. To achieve spatial accuracy and computational efficiency, we are continuing to develop adaptive gridding methods to resolve any spatially localized behavior, such as a flame. An important part of our program is the application of our work to practical problems, especially in chemical sciences and combustion.	10/01/85	09/30/86	435	450

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Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Science Applications International Corp	Alan Drobot/ Robert Gelinas	Moving Finite Elements in 2-D	This research project on moving finite element methods is focused on research and development of the method in two dimensions, including the development of research oriented software for solving systems of partial differential equations describing physical problems with shocks and moving fronts, such as in combustion processes. The project leadership was assumed by Drobot in 1985 with the purpose of concentrating on schemes for adding, removing, and reconnecting nodal points and gaining some understanding of the consequences on the physical accuracy of the solutions obtained. They offer to provide a listing of the moving finite element code as well as a users' manual. A manuscript on the properties of this method in 2D using a triangular grid should be available by the end of the contract.	04/15/81	07/31/85	65	36
Stanford University	George Dantzig/	Systems Optimization Project	Co-investigators on this project are R. W. Cottle, Walter Murray, and B. Curtis Eaves. Research associates are Philip Gill, Michael Saunders, Margaret Wright, and John Stone. Research topics include time staged linear programs, analysis of standard and ellipsoidal linear programming algorithms, methods for large scale linear complementarity problems, unconstrained optimization, constrained optimization, automatic scaling techniques, and simplified algorithms for solving dynamic multiregional planning models. The overall objective of the research is to develop effective methods for solving optimization (mathematical programming) problems. The areas of special concentration include staircase (dynamic) linear programs, large scale quadratic programming, nonlinearly constrained optimization (both dense and large scale), large scale energy-economic models, linear complementarity problems, and equilibrium problems.	11/01/83	10/31/86	300	315

Summary of Applied Mathematical Sciences Research Projects
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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of California, Berkeley	Jerrold Marsden/ Alan Weinstein	Stability of Fluids, Plasmas, and Nonlinear Wave Equations	The energy-Casimir method developed by the proposers, D. Holm, T. Ratiu and others will continue to be applied to a number of concrete fluid and plasma problems. Using these methods, free boundary problems will be investigated, as well as stratified flow. Related work will be carried out on averaging techniques and limits of projections of Hamiltonian structures, such as occur in BBGKY hierarchy to Maxwell-Vlasov and the Maxwell-Vlasov to charged fluid transitions. In addition, the proposers plan to use their techniques to study nonlinear wave equations in conjunction with the first year's planned visitor. Questions of stability, periodic solutions and chaos, (the latter using the Holmes-Marsden work on Melnikov's methods), will be considered. Melnikov's method is also expected to be useful in studying chaos for forced free boundary problems.	07/01/85	06/30/88	97	145
University of Illinois	C. W. Gear/ Robert Skeel	Computational Methods and Software for Ordinary Differential Equations	This work involves research on several open questions in the area of ODEs, viz., how to handle problems with multiple periods, why constant stepsize methods seem to work for certain classes of differential algebraic equations (DAEs), and how to handle general DAEs without prior symbolic analysis. Also, application of iterative methods to the solution of the nonlinear equations arising at each step in a stiff ODE or DAE and the effect of discontinuities on automatic stepsize methods will be studied. This rather broad scope covers the entire spectrum of problem areas encountered in solving energy related problems described by ODEs (and some classes of PDEs solvable by the Method of Lines).	11/16/83	11/15/86	184	194

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Maryland	James Yorke/ Edward Ott	Study of Chaotic Dynamics and Dimension of Strange Attractors	Faculty associate on this contract is Professor Sheldon Newhouse. Celso Grebogi is a research associate. Even simple mathematical models of physical systems are often observed to exhibit rather complex time evolution. In such situations the time evolution is often labeled "chaotic" or "turbulent." In many cases this chaotic behavior is associated with rather intricate, arbitrarily fine scaled, geometric structure of the attracting set to which a trajectory tends as the system evolves. These sets often possess Cantor set structure and are called "strange attractors." The study of strange attractors has recently undergone explosive growth. Motivation for this comes partly from the fact that strange attractors are being found to be of fundamental importance in many branches of science and engineering. Examples illustrating the wide ranging applications of strange attractors to physical and engineering problems are studies of turbulence in fluids, electrical circuits with tunnel diodes, buckling beams, plasma physics, lasers, solid state physics, magnetohydrodynamics, oscillations in the earth's magnetic field, chemically reacting systems, and many others. This program is to study two of the important aspects of strange attractors: the dimension of the strange attractors and how strange attractors evolve as a parameter is changed. Numerical experiments are a major tool in this study.	05/01/83	04/30/86	138	155

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Texas	David Young/ Graham Carey	Iterative Solution and Finite Element Analysis in Computational Mechanics	Co-investigators on this project are David Kincaid and Kamy Sepehrnoori. This project represents a research program embracing interrelated topics in applied mechanics, numerical analysis, and computer science. Specifically, we are investigating the theory and use of iterative solution algorithms in conjunction with finite element methods, for computing numerical solutions of certain classes of transient and nonlinear problems in mechanics and heat transfer that are of significant research and practical importance. Concurrently, we shall address related questions of accuracy and error estimates for finite element approximation and of stiffness and stability for semidiscrete systems in the transient problems. The actual solution of nonlinear mechanics problems, such as those encountered in Navier-Stokes problems, in reservoir simulation and in heat transfer with nonlinear chemical reactions will provide an assessment of new methodology arising from the research and for realistic applications. Finite element and iterative solution algorithms will be developed and evaluated for computations on supercomputers, vector processors as well as other advanced architectures. Part of the work involves a major expansion of the ITPACK library, with emphasis on improved vectorization and the use of special finite element methods adapted to vector computers. The suitability of certain types of iterative methods in conjunction with finite element methods for state of the art emerging parallel computing configurations is also to be studied.	08/01/84	07/31/87	135	155

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Washington	Jirair Kevorkian/	Resonance in Weakly Nonlinear Systems	Resonance is a common phenomenon in any physical process that involves coupled oscillations. In this research we consider recent work on nonlinear resonance in systems with slowly varying frequencies and indicate how this work applies to a quantitative description of the operation and stability of free electron lasers. Related to this is work in deriving adiabatic invariants for systems passing through resonance and work on wave propagation problems using multiple variable expansion techniques. In this project we will investigate the following areas: (1) A systematic analysis of free electron lasers including higher order effects and stability; (2) A study of nonlinear evolution equations as they occur in (1) or more generally in systems with strong interactions between modes; (3) The influence of nonlinear dissipation; and (4) Resonant wave interactions in unbounded media with slowly varying properties.	08/01/83	07/31/86	40	45
Virginia Polytechnic Institute & State University	Paul Zweifel/ William Greenberg	Applied Mathematics of Transport Theory	The goals of this research are to develop applicable mathematical techniques that are relevant to the physical transport processes underlying energy production. These include, for example, neutron transport, thermonuclear plasmas, rarefied gas dynamics, etc. Our concentration is on phonon and electron transport in solids, evaporation and condensation, study of abstract kinetic equations (existence and uniqueness theory), nonlinear plasma stability and acceleration and homogenization techniques in numerical transport theory calculations. Both analytical, function theoretical, techniques and numerical computations are planned.	02/01/83	11/30/86	51	92

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Washington State University	Kuruppu Ariyawansa/	Conic Algorithms for Unconstrained Minimization - Large Sparse Hessians	Existing algorithms for unconstrained minimization are based on local quadratic approximations. Local quadratic approximants cannot incorporate information on objective function values. Methods like DFP and BFGS that are successful for small dense problems cannot be fully extended to incorporate information on the structure of the Hessian in large sparse problems. These shortcomings are due to the limited degrees of freedom available in the quadratic model. The investigator has demonstrated that local conic approximations can be used to incorporate information on objective function values and to have the resulting algorithms possess good convergence properties. The objectives of the present research are three-fold. First we propose to continue the theoretical study of conic algorithms mentioned above to settle several issues necessary to implement these algorithms. Second, we propose to analyze a class of conic algorithms that includes complete conic extensions of DFP and BFGS methods for problems with sparse Hessians. Third, we propose to implement and thoroughly test several promising conic algorithms.	08/01/85	07/31/87	0	78

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Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Yale University	Tony Chan/	Efficient Numerical Methods for Large Nonlinear Systems	This project will study efficient numerical algorithms for solving large nonlinear systems that arise frequently in large scale scientific computing. In addition to general large nonlinear systems, we also consider problems with more inherent structures, including parameterized nonlinear systems that arise in homotopy and continuation methods and coupled nonlinear partial differential equations. The numerical techniques include multigrid and continuation methods, an approximate Newton method recently developed by the PI for solving coupled nonlinear systems and a nonlinearly preconditioned conjugate gradient method that does not require explicitly computing or storing the Jacobian. We will investigate the application of these methods to numerical continuation methods applied to the Navier-Stokes equations, the transonic flow equations and structural mechanics problems and to solving the coupled partial differential equations that arise in semiconductor device simulations. Finally, we will carry out the numerical implementations on the ELI CIRCUS, a ring of array processors being developed at Yale, and try to identify algorithmic implementations that can take advantage of the parallelism and vectorization capabilities provided by the architecture.	01/01/85	12/31/87	0	113

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
** Subtotal **						7128	7603
** Budget and Reporting Activity: KC 070102							
Brookhaven National Laboratory	Ronald Peierls/ Herbert Robbins	Statistical Methods	The primary emphasis of this research is on the development of innovative methodologies for analysis of data sets that are restricted, incomplete, or complex in other ways. A characteristic of such problems is that the observations to be analyzed are on subjects that are valuable, irreplaceable, and not easily reproducible. Such characteristics apply to weapons tests, nuclear reactors, large scale engineering structures and other systems of importance in energy and environmental research. To obtain reliable results from the analysis of the limited data sets associated with such exotic systems requires more sophisticated analysis than more conventional statistics, and is likely to call for extensive computation, both to implement these more sophisticated methods and also in their development through simulation and Monte Carlo methods.	10/01/85	09/30/86	343	275
Brookhaven National Laboratory	Ronald Peierls/ H. Bruce Stewart	Display and Analysis Systems	This task uses numerical simulation and computer visualization to understand qualitative behavior of nonlinear dynamical systems. The goal is to develop and implement new visual approaches to understanding topological structures in the phase space of a dynamical system. The methods are applied to differential equation models from structural and fluid mechanics, electromagnetics, chemical kinetics, and biological and ecological oscillations or fluctuations. Application of these phase space geometric analysis methods yields information about underlying order in apparently random fluctuating behavior (chaotic attractors) and changes of stability in dynamic behavior (bifurcations). Phase space geometric analysis is vastly enhanced by the use of interactive computer graphics. Current effort is directed toward designing software that tightly integrates the functions of dynamic simulation (solving differential equations), constructing systematic phase space portraits, and viewing and editing the resulting curves and surfaces.	10/01/85	09/30/86	0	25

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
George Washington University	James Foley/	Scientific Work Station Research	Scientific work stations, which are powerful networked personal computers with high quality graphics interfaces, are becoming an important tool for scientists to use in their daily computational, information management, and communications work. This research centers on several issues where progress will help increase the productivity, usability, programmability, and efficiency of these work stations. The research topics are: development and testing of a graphics interface to the work station and network operating system to augment current text oriented interfaces; development of a "look up table compiler" language as part of our work on device independent graphics for raster displays; and development of an object oriented graphics programming language and language implementation suited for use in the next generation of multiprocessor scientific work stations.	08/01/83	07/31/86	55	60
Lawrence Berkeley Laboratory	Carl Quong/ Arie Shoshani	Large Scale Scientific Data Management Research	The data management research program is aimed at the development of specialized data management techniques for scientific and statistical databases. Scientific databases result from experiments and simulations of physical phenomena, such as the collision of particle beams or modeling fluid dynamics systems. Statistical databases are collected primarily for the purpose of providing statistical summaries, such as energy consumption and production. These databases have characteristics that cannot be supported efficiently by existing commercial data management systems. The purpose of the data management research program is twofold: to identify the special characteristics and problems that exist in scientific and statistical databases, and to develop techniques that are tailored to the special structures and usage of such databases. Special emphasis is placed on techniques that can take advantage of parallel processing opportunities.	10/01/85	09/30/86	500	525

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Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Oak Ridge National Laboratory	Robert Ward/ Toby Mitchell	Statistical Methods	The statistical methods research effort is divided between the computational statistics (CS) and analysis of large data sets (ALDS) research projects. Research in the CS project will include work in computer aided experimental design, algorithms for computing distributional properties of estimators and test statistics, iteratively reweighted least squares algorithms, computational aspects of large scale regression problems requiring sparse matrix technology, and algorithms for computing Bayesian posterior distributions. Since most of these algorithms are computationally intensive, special emphasis will be placed on their implementation using parallel processing. Research in the ALDS project will focus on the following areas: evaluation of the effect of data transformation on misclassification probabilities in multivariate discriminant analysis; investigation of Bayesian variable selection methods along with the development of the necessary computer algorithms for computation of posterior distributions of interest; and development of methods to analyze data arising from imperfect sampling frames.	10/01/85	09/30/86	365	360

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Pacific Northwest Laboratory/ Battelle	Wesley Nicholson/ Marvin Erickson	Analysis of Large Data Sets	Effectively utilizing the growing quantities of complex energy related data requires new techniques in data analysis, data display, and data management. This integrated statistics and computer science research project is supported by the research computing facility, a statistical laboratory that serves as a testbed for new methods of and approaches to analysis. Specific topics addressed in graphical analysis research are 1) new techniques for increasing the number of points and dimensions that can be displayed and manipulated, and 2) the definition and automatic detection of "interesting" structure. Data analysis management research focuses on the management and control of 1) information generated by the analysis process (derived data) and 2) information concerning the analyst's interpretation of results. The specific issues that we will address are automated structure detection in large multivariate data sets and the applicability of supercomputers for these calculations.	10/01/85	09/30/86	500	400
University of Florida	Stanley Su/	A Dynamic Multicomputer System for Managing Scientific and Engineering Data	This research project entails the design, analysis, and evaluation of a multicomputer system that consists of multiple processors on a dynamically partitionable network with switchable main memory modules. They will investigate the architectural features of this system suitable for parallel processing of numerical and symbolic data for scientific and engineering databases common in energy research and applications. The design and evaluation of software algorithms that take advantage of these architectural features will be undertaken.	08/01/84	07/31/86	81	85

Summary of Applied Mathematical Sciences Research Projects
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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Utah	Robert Barnhill/	Computer Aided Surface Representation	Faculty associates on the project are P. Alfeld, G. Farin, and A. Worsey. The aims of this research project are the creation of new surface forms and the determination of geometric and physical properties of surfaces. The investigation of new surface forms include the topics of piecewise polynomial triangular interpolants, monotone and convex surfaces, closed and convolution surfaces, tetrahedral interpolants, surfaces defined on surfaces, and a multidimensional Coons' patch (Gregory's Cube). The geometric and physical properties considered include the estimation of derivative data, numerical integration, contouring, and the tesselation of points in 3D. The surfaces to be created must satisfy a variety of criteria such as sufficient smoothness, reasonable shape, and sufficient accuracy or fidelity. We take the approach of developing a robust class of surfaces that can utilize arbitrarily located information that is frequently demanded in DOE applications. This approach is particularly difficult for multidimensional interpolation to data in three or more variables. The parallel rendering of surfaces will be investigated.	06/01/85	05/31/88	132	307

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Washington	Werner Stuetzle/ Andreas Buja	Nonparametric Methods in Multivariate Analysis	The principal goal of this research is the creation of new statistical tools to explore the structure of large scientific data sets. An initial focus of this work will be the detection of nonlinear relations amongst predictor and response data, where the response is a separable or additive function of the predictor variables. The problems to be studied involve the optimal determination of the separable response functions, a computationally intensive problem. A second area is the determination of whether the predictions obtained from a given data analysis are degenerate. This work generalizes the search for linear dependencies in classical regression analyses. In addition to the development of analytical models, the investigators will develop sophisticated graphics capabilities to explore the structure of large scientific data sets and assess model predictions generated computationally.	07/01/85	06/30/88	0	250
University of Wisconsin	David DeWitt/ Douglas Bates	Database Machines for Large Statistical Databases	This project will investigate the issues involved in the design of a high performance statistical database machine. One task is to perform a static and dynamic analysis of the principal statistical operations to determine the frequency of use of primitive linear algebra building blocks, such as matrix multiplication and inversion. The second task is the implementation of a relational dataflow database machine, called FLASH, on the reconfigurable multiprocessor hardware called CRYSTAL. FLASH will be modified to incorporate the linear algebra building blocks as new query processor primitive operations. The resulting system will be monitored as it is used by staff and students in the University of Wisconsin Statlab for the purpose of gathering statistics on various system performance parameters such as disk traffic, communications traffic among the various components, and utilization and consumption of resources by the linear algebra building blocks selected. A benchmark relational database will be developed and a set of benchmark queries will be designed to quantify performance features of various algorithms on various architectures in the context of a large statistical database.	01/16/83	01/15/86	86	121

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
** Subtotal **						2062	2408
** Budget and Reporting Activity: KC 070103							
Argonne National Laboratory	Paul Messina/	Advanced Computer Systems Concepts	Research in automated reasoning plays a major role in our software engineering activities. Studies include development of an abstract machine for logic programming, design of new inference rules and strategies, and applications to problems of interest to DOE. A second major focus is advanced scientific computing. This program comprises the establishment of an advanced computer research facility and the development of a broad research program in mathematics and computer science. The goal is to understand and express the level of parallelism possible in numerical and nonnumerical tasks and to exploit the strengths of particular architectures. In addition, Argonne is working on applications of software engineering techniques to the production of program packages like MINPACK; abstract programming; and standards for Fortran, PL/I, and IEEE floating point arithmetic. New work includes design of simplification transformations for our automated program transformation system and creation of a unified package for eigenvalues and systems of linear equations.	10/01/85	09/30/86	1085	1950

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
California Institute of Technology	Geoffrey Fox/	The Caltech Concurrent Computation Program	Associated faculty on this project are Aron Kupperman, Rob Clayton, Herbert Keller, Philip Saffman, R. Blandford, N. Corngold, R. Gould, P. Haff, B. Hager, P. Liewer, and T. Tombrello. The Caltech Concurrent Computation Project (CCCP) is a new approach to homogeneous architectures begun in the Caltech Cosmic Cube Project. An important lesson learned from that project is the importance of having a significant amount of computational power in each of the nodes (including a large enough memory local to the node to contain a significant computational problem) and the effectiveness of offloading the communication processes to coprocessors, including broadcast capabilities. The new nodes proposed, built from off the shelf components available from the vendors, will have these important features. In particular, the independent communication coprocessors should be capable of demonstrating the scalability of the hypercube architecture to much larger machines and also the feasibility of using heterogeneous processors in a hypercube configuration. They should be able to demonstrate true MIMD capability with this new processor node. The broad spectrum of scientific disciplines represented in this project is extraordinary (possibly unique). They have been successful in demonstrating techniques for mapping a long series of computational methods onto the hypercube architecture. Given the importance to DOE research and development programs of future parallel architectures for supercomputers, the Caltech project has pioneered a novel method for analyzing the structure of scientific models and devising new (and revising old) parallel algorithms to maximize the efficient use of these new machines.	08/01/85	07/31/90	900	1400

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Lawrence Berkeley Laboratory	Carl Quong/ Joseph Sventek	Advanced Computer Concepts	The advanced computer concepts program concentrates on the understanding and resolution of problems that prevent the effective use of distributed computer systems. One major thrust of the program is the performance measurement of local area network (LAN) hardware, performance measurement of communication protocol implementations using this hardware, and subsequent analysis of the measurements using simulation and other modeling techniques. This work will lead to realistic estimates of LAN performance in DOE environments; in addition, the enhancements to network hardware and software necessary to achieve required performance characteristics can be determined. A second major research area involves distributed computing and network access in DOE environments. The design and development of scientific workstations is the primary focus, with special emphasis upon their integration with existing local computational facilities and the Energy Research supercomputer network. The activities range from application software design for existing workstation computers to the design and implementation of a distributed file system for heterogeneous environments to software to gateway between different transport level protocols. The ultimate goal of this work is to permit scientists to use all of the computational tools at their disposal from within an environment tailored to their needs.	10/01/85	09/30/86	300	315

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Lawrence Livermore National Laboratory	Robert Huddleston/ James McGraw	Advanced Computing Concepts	Research in advanced computing concepts focuses on algorithm and language development and implementation as well as efficient programming techniques in a multitasking, multiprocessing computational environment. New research is planned in parallel algorithm design for solving multiple scales problems, in developing and implementing multitasking techniques for large scale numerical models applicable to various multitasking configurations, and in automated programming for numerical simulation systems. Research will continue in modeling and analysis of multiple scales problems, the numerical solution of PDEs arising from multiple scales problems, the numerical solution of systems of linear equations, algorithms and language development suitable for parallel and vector processors, and algorithm development for solving hydrodynamics problems.	10/01/85	09/30/86	450	555
Los Alamos National Laboratory	Norman Morse/	Advanced Computational Concepts	Serious efforts to overcome the speed limitations inherent in single processor computers have invariably involved parallel processing. The next generation of commerical supercomputers will all be shared memory parallel machines having from 8 to 16 very fast (probably vector) processors. Efficient utilization of these machines will require some significant changes in the techniques used in code development. Different algorithms will have to be created and in some cases, new mathematical models, languages, and techniques developed. In the more distant future, massively parallel machines have been proposed, consisting of hundreds and even thousands of processors to be applied to a single problem. Los Alamos has been actively involved in parallel processing for over four years, having obtained seminal results on parallel processing of applications codes. This project consists of research activities in the areas of experimental equipment, algorithm development, language research, and computational modeling methodology for parallel applications.	10/01/85	09/30/86	700	735

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Massachusetts Institute of Technology	Edward Fredkin/	Information Preserving Models of Physics and Computation	The Information Mechanics Group in MIT's Laboratory for Computer Science is developing the field of information mechanics, which deals with dynamical systems that can be thought of either as models of idealized physical processes or as physical models of computational processes. These systems are derived from conventional models of computation by adding contraints to bring the models into better agreement with physical principles; or they can be derived from conventional models of physical processes by introducing certain assumptions that are required for finitary computational models. The basic assumptions of information mechanics are: (a) the structure and the laws of dynamical systems are such that their evolution can be computed exactly by finite means, and (b) the laws that govern the evolution of these dynamical systems are exactly reversible (i. e., characterized by an invertible law, not necessarily a law that is invariant under time reversal). The second point implies that information is conserved in the evolution of the system. The investigators propose to apply these ideas to simulate physical processes involving exponential decay, turbulence, and in general, Hamiltonian dynamical systems. Simulators can be implemented with specially designed VLSI chips that give orders of magnitude speed up over general purpose computers. These ideas may provide valuable insight into the nature of reversible, discrete models of physics and computation.	07/15/83	07/14/86	110	121

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Massachusetts Institute of Technology	Jack Dennis/	High Performance Data Flow Computers	This research effort investigates the data flow approach to high performance computer systems through six closely related projects: language development, prototype evaluation facility, program translation, data structures, architecture description and simulation, and specification of a full scale data flow processor. The language development project seeks to develop a user oriented higher level language that provides a mechanism for specifying an algorithm that can be translated into a form of directed graphs. The VAL language has been developed for this purpose. The prototype evaluation facility allows the design of a machine instruction set that is suitable for representing the directed graphs of the data flow machine. The program translation project will provide tools for translating from the user language, VAL, to the machine instruction set. The data structures project will provide data structures supporting the data flow concepts and which are useful for numerical computations. The architecture description and simulation project provides tools for the analysis of possible implementations of data flow machines. The specification project will summarize conclusions about the applicability of the data flow concepts to typical large scientific and engineering codes.	01/01/85	12/31/85	231	280

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
New York University, Courant Institute	Peter D. Lax/ Malvin Kalos	Advanced Computing Concepts: the Ultracomputer Project	Jack Schwartz and Alan Gottlieb are investigators on this project. This project entails the study of architectures for highly parallel computing systems, perhaps comprising many thousands of tightly coupled high performance microcomputers. Machines of this type could develop compute rates several hundreds of times larger than today's most powerful machines. Using such new machines efficiently will require developing new types of operating systems and adapting existing programming methods and languages. Effective, highly parallel coordination techniques are particularly important if efficiency is not to be lost. Machines of this power can play a central role in meeting DOE requirements for large scale computing. Significant joint research with IBM has begun on a parallel processor architecture called the RP3 that is based on ultracomputer principles. It is likely that a 16 processor prototype will appear at the beginning of 1986 and a 512 processor prototype could appear in 1987. We expect to enhance our program to respond to the opportunities implicit in this development. Specifically, we will propose to acquire one of each prototype and prepare for their use here and, through networking, by the entire DOE computational research community.	10/01/85	09/30/86	660	1188

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Colorado	Leon Osterweil/	Integrated Testing and Analysis of Mathematical Software Tools	The associated investigators on this project are Dieter Boecher and John Shultis. The Toolpack project that preceded this project was a joint effort of the University of Colorado, Argonne National Laboratory, University of Arizona, NAG, LTD., and Purdue University. The prototype Toolpack system developed under the original contract is being distributed by the National Energy Software Center at Argonne and by NAG, LTD. This project will build a well integrated ensemble of testing and analysis software tools based on an augmented Toolpack/IST system. Graphics tools for aiding in the analysis and debugging of mathematical software will be developed and tested. The design of graphical analysis and display tools is of particular importance to DOE for mathematical modeling software development. The research is focused on analytical displays of program development environments on scientific workstations. The complementary use of instrumentation and analysis could provide an effective framework for organizing and conceptualizing the orderly and systematic process of program verification.	08/01/84	07/31/87	175	145

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Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Illinois	David Kuck/ Duncan Lawrie	Center for Supercomputing Research and Development (CEDAR)	Ahmed Sameh and Edward Davidson are co-investigators on this project. This grant supports research in computer science and architecture, software, and algorithms and applications for the CEDAR architecture. The goals of this three year effort are to demonstrate the operation of an experimental research computer with the CEDAR architecture, complete with the optimizing, structure analyzing compiler based on Parafrase and KAP, new problem decomposition techniques, and algorithms applicable to large scale scientific computation relevant to DOE mission programs. The three components of the project are as follows. Hardware: In year one, two clusters will be purchased from a suitable vendor and connected in some suitable manner such that a two cluster system will be available for use in the project. During year two, two prototype boards will be designed and fabricated that will allow for the connection of up to eight clusters in a general way so as to support CEDAR implementation of software. By the beginning of year three the original two cluster system will be connected to provide a four cluster operational CEDAR experimental machine. During year three a larger multilevel switch capable of supporting up to 1024 processors will be designed. At this point the advisability of purchasing more clusters can be determined. Software: In year one a working prototype of the optimizing compiler based on Parafrase will be available. A production compiler based on KAP but specialized to the CEDAR architecture should be ready by the first quarter of year two. Development of the KAP based compiler will continue throughout the life of the project. Algorithms and Applications: Performance of nine applications selected by project researchers will be measured on the various versions of the CEDAR machine as the project proceeds. This will be an ongoing effort and will include work by collaborators (such as staff from Argonne) as well as the CEDAR staff.	02/15/85	02/14/88	226	2300

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Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
University of Texas	James Browne/ Clement Leung	A Unified Approach to Parallel Computation	Components of this research project are: the construction and evaluation of a simulation modeling system for parallel computation structures; the development of an architecturally independent programming system; and investigation of a formulation support environment for parallel computation. Proposed work on systematic development of algorithmically specialized architectures may be investigated if the time and budget constraints allow. Preliminary work on the Computational Structures Language demonstrated the usefulness of abstracting parallel programming constructs in a formalism that allows analysis of algorithms in terms of computational units, communication structures, and synchronization primitives. This is a viable approach to determining the relative efficiencies of mapping equivalent algorithms devised to solve a computational problem onto various parallel architectures - that is, it provides a formal mechanism for "benchmarking" problems on different architectures without having to specify a particular language or implementation strategy a priori.	09/01/85	08/31/88	123	196

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
** Subtotal **						4960	9189
** Budget and Reporting Activity: KC 070200							
Ames Laboratory, Iowa State University	James Corones/	Network Access and Research Computing Facility	Network access includes the operation and maintenance of a Vax 11/750, graphics workstation, and a link to the laboratory's Vax/FPS 164 facilities.	10/01/85	09/30/86	0	25
Argonne National Laboratory	Paul Messina/	Energy Sciences Advanced Computation	The network access activity encompasses three projects aimed at providing access to supercomputers and computer network facilities for Energy Research programs: (1) the Energy Research supercomputer network gateway facility, (2) the massively parallel supercomputer center, and (3) Argonne's research computing facility. Work has just begun on the first two activities; the research computing facility continues to provide a computing environment tailored to mathematical and computer science research.	10/01/85	09/30/86	100	225
Brookhaven National Laboratory	Ronald Peierls/	Network Access	Network access includes a 50 KB link to the NYU TAC.	10/01/85	09/30/86	0	25

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Florida State University	Joseph Lannutti	Supercomputer Computations Research Institute	The Supercomputer Computations Research Institute conducts research in computational sciences, including physics, chemistry, geophysics, oceanography, applied mathematics, and others. Supercomputer access is provided to on site researchers and to other qualified OER researchers through the national MMFECC network.	10/01/84	09/30/89	0	7000
Lawrence Berkeley Laboratory	Carl Quong/ Joseph Sventek	Network Access	Network access activity provides the computational resources needed to support the Laboratory's basic research program in Applied Mathematical Sciences. Maintenance and improvement of the local research computing facilities which provide the standard functions such as program development, electronic mail, network access, document preparation, text processing, high quality graphics, etc., will continue. Additionally, special attention will be directed toward the problems of remote access to the ER supercomputer network through local computational facilities which provide an integrated computing environment to the user.	10/01/85	09/30/86	100	100
Lawrence Livermore National Laboratory	John Killeen/	National Magnetic Fusion Energy Computer Center and Network	This reflects the portion of the MMFECC budget that provides supercomputer access to the non-MFE researchers in ER, including network access, upgrade of ports at ER sites (SLAC, Fermi, ANL, LBL, and others).	10/01/85	09/30/86	100	5943

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Los Alamos National Laboratory	Billy Buzbee/ David Campbell	Workshops in Computing and Mathematical Sciences	Each year the Los Alamos Computing Division and the Center for Nonlinear Studies host a series of workshops addressing leading issues in computing and mathematical sciences. The purpose of this program is to help defray associated costs. Costs of these workshops include publication (agendas, abstracts, proceedings), and travel support for speakers.	10/01/85	09/30/86	100	100
New York University, Courant Institute	Peter D. Lax/ Max Goldstein	Research Computing Facility and Network Access	The research computing facility provides the computational resources needed to support the ongoing basic research in Applied Mathematical Sciences. It serves as a testbed for the evaluation and deployment of new computing capabilities. Maintenance and development of this facility, including integration and evaluation of emerging computing technologies, is a focal point for collaborative interaction with other DOE research sites and with researchers in computer science throughout the university and industrial communities. The experimental effort places special emphasis on issues related to distributed computing environments and the applicability of varied computational resources to DOE scientific researchers. The goals of the experimentation are to: (a) provide a variety of computer facilities to the CMCL community; (b) acquire and devise means to easily enable communications among the various hardware and software elements comprising the research facility; and (c) discover and implement means that reduce the impact on the user of the complexity inherent in multicomputer environments.	10/01/85	09/30/86	150	150

Summary of Applied Mathematical Sciences Research Projects
Fiscal Years 1984 and 1985

Institution	Project Manager/ Investigator(s)	Title of Project	Summary of Project in FY 1985	Start Date	End Date	FY 84 ($000)	FY 85 ($000)
Oak Ridge National Laboratory	Robert Ward/	Research Computing Facility and Network Access	The network access task provides for the improvement, operation, and maintenance of a research computing facility for the Mathematical Sciences section. The principal item in our facility is a DEC Vax 11/780 acquired late in FY 1983. Connection to the Defense Data Network (Milnet/Arpanet) took place in 1984. This facility will continue to be upgraded and be used to explore innovative approaches to scientific computing and to communicate with researchers at other DOE facilities. It is anticipated that this facility will also serve as the network gateway to an experimental prototype parallel computer to be acquired in FY 1985.	10/01/85	09/30/86	75	100
Pacific Northwest Laboratory/ Battelle	Marvin Erickson/ Wesley Nicholson	Network Access and Research Computing Facility	The research computing facility is operated and maintained for use by Applied Mathematical Sciences researchers.	10/01/85	09/30/86	0	100

DOE/ER-0158/2
Dist. Category UC-38

Summaries of FY 1984 Engineering Research

December 1984

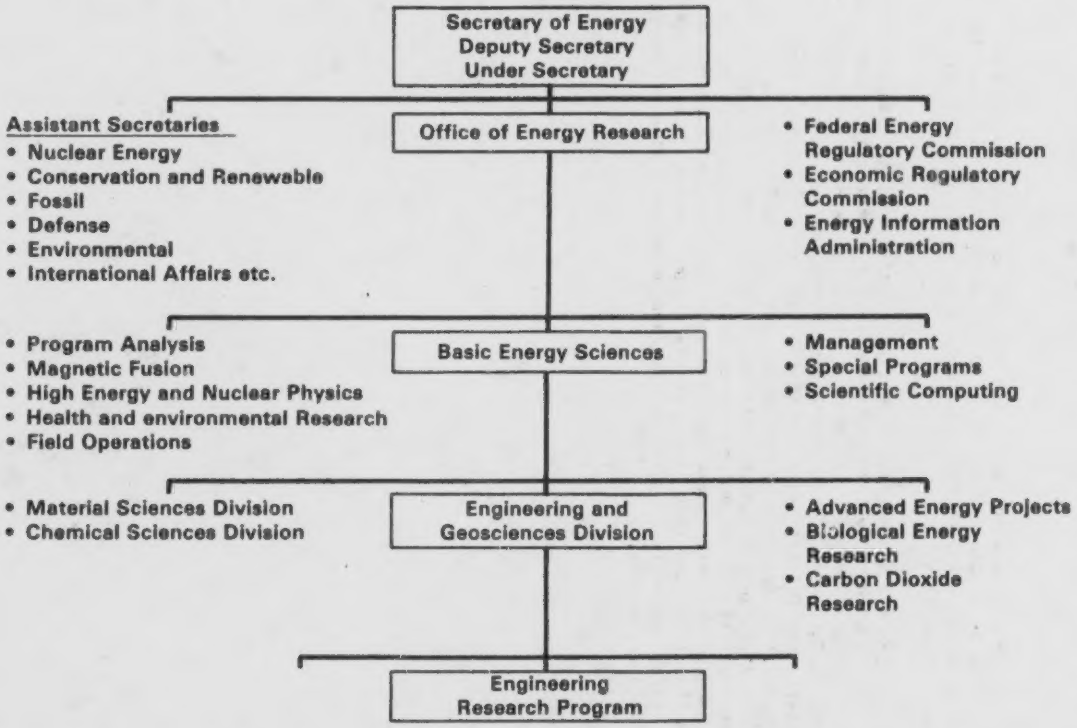
U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Engineering and Geosciences
Washington, D.C. 20545

FOREWORD

This report documents the BES Engineering Research program for fiscal year 1984; it provides a summary for each of the program projects in addition to a brief program overview. The report is intended to provide staff of Congressional committees, other executive departments, and other DOE offices with substantive program information so as to facilitate governmental overview and coordination of Federal research programs. Of equal importance, its availability facilitates communication of program information to interested research engineers and scientists. The organizational chart for the DOE Office of Energy Research (OER) on the next page delineates the six Divisions within the OER Office of Basic Energy Sciences (BES). Each BES Division administers basic, mission oriented research programs in the area indicated by its title. The BES Engineering Research program is one such program; it is administered by the Engineering, and Geosciences Division of BES. Dr. Oscar P. Manley is technical manager of the Engineering Research program; inquiries concerning the program may be addressed to him, in writing or by phone at (301) 353-5822.

In preparing this report we asked the principal investigators to submit summaries for their projects that were specifically applicable to fiscal year 1984. The summaries received have been edited as necessary, but the press for timely publication made it impractical to have the investigators review and approve the summaries prior to publication. For more information about a given project, it is suggested that the investigators be contacted directly.

Engineering Research Program within DOE


Secretary of Energy
Deputy Secretary
Under Secretary
Assistant Secretaries
• Nuclear Energy
• Conservation and Renewable
• Fossil
• Defense
• Environmental
• International Affairs etc.
Office of Energy Research
• Federal Energy Regulatory Commission
• Economic Regulatory Commission
• Energy Information Administration
• Program Analysis
• Magnetic Fusion
• High Energy and Nuclear Physics
• Health and environmental Research
• Field Operations
Basic Energy Sciences
• Management
• Special Programs
• Scientific Computing
• Material Sciences Division
• Chemical Sciences Division
Engineering and Geosciences Division
• Advanced Energy Projects
• Biological Energy Research
• Carbon Dioxide Research
Engineering Research Program

INTRODUCTION

The individual project summaries follow the program overview. The summaries are ordered alphabetically by name of institution and so the table of contents lists all of the institutions at which projects were sponsored in fiscal year 1984.

The projects are numbered sequentially for individual identification in the indexes. Each project entry begins with a centered, institutional-departmental heading. The project number precedes the capitalized project title. The names of the investigators are listed immediately below the title. The funding level for fiscal year 1984 appears to the right of the title; it is followed by the budget activity number (e.g., 01-03). These numbers categorize the projects for budgetary purposes and the categories are described in the budget number index. The year in which the project began and the anticipated duration in years are indicated respectively by the first two and last digits of the sequence directly below the budget activity number (e.g., 82-02). The summary description of the project completes the entry.

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PROGRAM REVIEW

BES ENGINEERING RESEARCH

The BES Engineering Research program is one of the component research programs which collectively constitute the DOE Basic Energy Sciences program. The DOE Basic Energy Sciences program supports energy related research in the physical and biological sciences, engineering, and applied mathematics. The chief purpose of the DOE Basic Energy Sciences program is to provide the fundamental scientific base on which identification and development of future, national energy options will depend. The major product of the program becomes part of the body of data and knowledge upon which the applied energy technologies are founded; the product is knowledge relevant to energy exploration, production, conversion and use.

The BES Engineering Research program was started in 1979 to help resolve the numerous serious engineering issues arising from efforts to meet U.S. energy needs. The program supports fundamental research on broad, generic topics in energy related engineering--topics not as narrowly scoped as those addressed by the shorter term engineering research projects sponsored by the various DOE technology programs. Special emphasis is placed on projects which, if successfully concluded, will benefit more than one energy technology. During the first year several workshops were sponsored for the purpose of identifying energy related engineering research needs and initial priorities. Representatives from industry, academic institutions, national laboratories, and leading members of professional organizations (Engineering Societies Commission on Energy, American Society of Mechanical Engineers, Society of Automotive Engineers, and Joint Automation and Control Committee) participated in the workshops. In addition to the participants in the workshops, staff representatives from the DOE technology programs and other leading U.S. energy engineering experts made significant contributions to the setting of program priorities. There resulted from this process a strong confirmation of the need for a long-range, fundamental engineering research program with two major goals. The broad goals that were established by this process for the BES Engineering Research program are:

1) To extend the body of knowledge underlying current engineering practice so as to create new options for enhancing energy savings and production, for prolonging useful equipment life, and for reducing costs without degradation of industrial production and performance quality; and

2) To broaden the technical and conceptual base for solving future engineering problems in the energy technologies.

In this process, it was further established that to achieve these goals, the BES Engineering Research program should address the following topics identified as essential to the progress of many energy technologies:

1) Advanced Industrial Technology — improvement of energy conversion and utilization, opening new technological possibilities, and improvement of energy systems.

2) Fluid Dynamics and Thermal Processes -- broadening of understanding of heat transfer in non-steady flows, methodology for reducing vibrations and noise in heat exchangers, and engineering aspects of combustion.

3) Solid Mechanics -- continuum mechanics and crack propagation in structures.

4) Dynamics and Control of Processes and Systems -- development and use of information describing system behavior (system models), performance criteria, and theories of control optimization to achieve the best possible system performance subject to known constraints.

In addition to the above topics, Geotechnical Engineering (mining), Electric Power Technology, Reliability and Risk Analysis, and Novel Energy Related Engineering were endorsed as areas suitable for immediate initiation of engineering research projects. Because of budgetary limitations, the implemented BES Engineering Research program is somewhat less broad than the program envisioned above. At present, equal emphasis is being placed on three carefully selected, high priority research areas; namely,

1) Mechanical Sciences -- including tribology (basic nature of friction reduction phenomena), heat transfer, and solid mechanics (continuum mechanics and crack propagation).

2) System Sciences -- including process control and instrumentation.

3) Engineering Analysis -- including non-linear dynamics, data bases for thermophysical properties of fluids, and modeling of combustion processes for engineering application.

These areas contain the most critical elements of the four topics enumerated above; as such they are of importance to energy technologies both in the short and long term, and therefore of immediate programmatic interest. It should be noted that other areas of basic research important to engineering are monitored elsewhere in BES. For instance, separation sciences and research on thermophysical properties, are among the responsibilities of the Chemical Sciences Division, while microscopic aspects of fracture mechanics are in the domain of the Material Sciences Division. As resources permit, other high priority areas are being added to the Engineering Research program. Thus as a result of some growth in the program budget an important development has taken place in the Engineering Research Program: two major concentrations of research were initiated. First, a new program was organized at Oak Ridge National Lab dealing with intelligent machines in unstructured environment (see page 53). It is expected that some resources will be available for coordinated, more narrowly focussed related, high quality research at universities and other research centers. All such activities will be supported and administered directly by the Engineering Research Program, but some coordination of efforts with the ORNL program may prove useful. The research opportunities in this area of interest to the DOE - Engineering Research Program have been identified in a workshop held in November, 1983. Proceeding of the workshop entitled "Research Needs in Intelligent Machines" are available from the Center for Engineering Advanced Systems Research, Oak Ridge National Lab, Post Office Box X, Oak Ridge, TN, 37830.

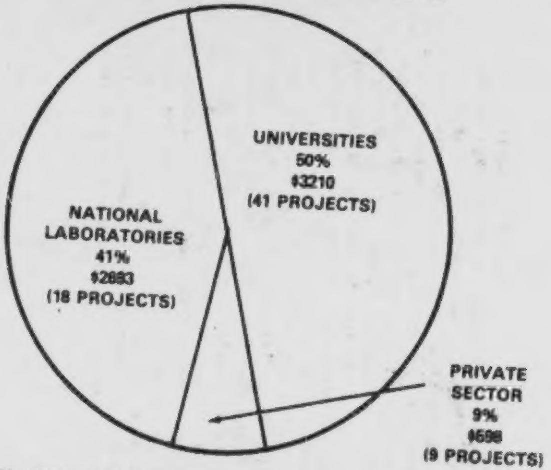
Secondly in FY 1985 there has started a collaborative research effort between MIT and Idaho National Engineering Lab. At present, the collaboration is in four distinct areas: Plasma Process Engineering, Automated Welding, Fracture Mechanics, and Advanced Engineering Methods and Analysis.

Again, it is expected that colateral, high-quality research efforts at other institutions will be supported by the Engineering Research program.

Finally, it should be mentioned that some very limited support is expected in FY 1985 for research on large scale systems. A report of a Workshop on Needs, Opportunities, and Options in this field is available from Professor G. L. Thompson, Graduate School of Industrial Administration, Carnegie-Mellon University, Pittsburgh, PA, 15213.

Research projects sponsored by the BES Engineering Research program are currently underway at universities, private sector laboratories, and DOE national laboratories. In fiscal year 1984 the program operating funds available amounted to about $6.5 million. The distribution of these funds among various institutions and by topical areas is illustrated on the next page. Project funding levels are mostly in the range of $50,000 to $100,000 per year. Typical duration of a project is three to four years, with some projects expected to last as long as ten years or more. The BES Engineering Research projects stem almost without exception from unsolicited proposals. Proposals which anticipate definite results in less than two years are usually referred to the appropriate DOE technology program for consideration. Anyone interested in submitting a proposal is encouraged to discuss his ideas with the technical program manager prior to submission of a formal proposal. Such discussion helps to establish whether or not a potential project has a reasonable chance of being funded. The primary considerations for possible support are the technical quality of the proposal and the professional standing of the principal investigators and staff. An effort is made to attract first rate, younger research engineers and energy oriented applied scientists. A high technical caliber of research is maintained by requiring that the projects supported have potential for a significant contribution to energy-related engineering science, or for an initial contribution to a new energy relevant technology. Sponsored projects are selected primarily for their relevance to DOE mission requirements; the contribution to energy related higher education is an important but secondary consideration. Thus projects sponsored at universities are essentially limited to advanced studies both theoretical and experimental usually performed by faculty members, staff research scientists, and doctoral candidates.

ENGINEERING RESEARCH PROGRAM
FY '84 BUDGET ($000's)
BY INSTITUTIONAL TYPE



ENGINEERING RESEARCH PROGRAM
FY '84 BUDGET
BY TECHNICAL AREAS

	($000 s)	%	NUMBER OF PROJECTS
MECHANICAL SCIENCES	1694	26	23
SYSTEMS SCIENCES	2694	41	21
ENGINEERING ANALYSIS	2113	33	24

AMES LABORATORY
Iowa State University
Ames, Iowa 50011

01. A COMPOSITE, MULTIVIEWING $200,000 01-03
TRANSDUCER 81-3
D. O. Thompson

The objective of this project is to demonstrate a composite, multiviewing ultrasonic transducer suitable for detecting, characterizing, and reconstructing flaws in structural materials for various applications. Development of this transducer utilizes a combination of recent advances in ultrasonic scattering and inversion theories with new concepts in transducer configurations and excitation methods. An experimental model of a composite transducer has been used as an aid in developing the semiautomated data acquisition and protocol. It has been determined that seven transducer elements which are multiplexed using both pulse-echo and pitch-catch modes are sufficient to produce good flaw reconstructions. Effects of limited aperture on the reconstruction have also been examined. The reconstruction protocol fits the acquired data to an "equivalent" ellipsoid of general shape (3 axes, 3 angles), a shape that is compatible with a fracture mechanics description of growing flaws and thus suitable for failure prediction. Criteria have also been established for individual transducer selection using experimentally determined scattering results. It is suggested that this procedure may form an approach for the further development of new transducer standards.

ARGONNE NATIONAL LABORATORY
Components Technology Division
Argonne, Illinois 60439

02. THEORETICAL/EXPERIMENTAL STUDY $120,000 01-02
OF STABILITY CONTROL 82-3
S. S. Chen, E. L. Reiss (Northwestern U),

Theoretical and experimental studies are aimed at enhancing the understanding of nonlinear stability phenomena involving fluids, solids, and their coupling. The objective is to develop methods of controlling instability, and to explore the use of instability mechanics in engineering design. Studies of the mathematics of the modeled nonlinear systems are conducted at Northwestern University. Experiments and related analysis are performed at Argonne National Laboratory. Studies have been performed on the special fluidelastic stability problem of a slender elastic tube conveying fluid. In order to develop the required mathematical techniques and to understand the mathematical and physical phenomena that may occur, simpler oscillator problems have been studied. These include two simple, coupled nonlinear oscillators as a model to study nonlinear stability control by secondary bifurcation and to develop a technique to study subcritical bifurcation. In parallel with the theoretical study, experiments have been performed with a tube, fixed at the upstream end and supported at a downstream location by a knife-edge support whose distance from the end can be varied. A series of tests has been performed and reported. In addition, a numerical technique to predict large-amplitude oscillations above the critical flow velocity has been developed; numerical results agree well with experimental data. Further studies will focus on the analytical method for subcritical bifurcation, stability of channel flow and tests to understand the existence and control of chaotic motion in a mechanical system.

ARGONNE NATIONAL LABORATORY
Components Technology Division
Argonne, Illinois 60439

03. BOUNDS ON DYNAMIC PLASTIC DEFORMATION $50,000 01-03
C. K. Youngdahl 84-3

In many applications where load is transmitted to the structure through a fluid, details of the load history and spatial distribution affect significantly the final plastic deformation. The objective of this project is to devise load correlation parameters based on various weighted integrals of the time-space load distributions which can be used to characterize the effects of the load without resorting to detailed numerical analysis. These load correlation parameters have three important uses: to perform design and safety analyses of structures over a wide range of design variables and loadings; to validate computer programs which have a nonlinear dynamic plasticity capability; and to correlate experimental simulations with actual or predicted events. The dynamic plastic deformation of some basic structural configurations will be analyzed for loadings which vary both in magnitude and region of application with time. Load correlation parameters will be hypothesized and their usefulness in predicting final plastic deformation will be determined. The analyses will be based initially on a rigid, perfectly plastic material model, but will be extended to include strain hardening and elastic effects if the work to determine load parameters is successful.

BATTELLE-COLUMBUS LABORATORIES
Physical Metallurgy Section
505 King Avenue
Columbus, Ohio 43201

04.	DAMAGE ACCUMULATION BY CRACK GROWTH UNDER COMBINED CREEP AND FATIGUE C. E. Jaske	$56,000	01-04 83-3

The objective of this study is to develop and evaluate methods for assessing creep/fatigue crack growth under inelastic straining. A fracture-mechanics approach implementing the J integral for fatigue and the C* integral for creep is being employed A crack-tip-zone interaction model is used to account for the interactions between creep and fatigue during crack growth at high temperatures. Experimental studies on Type 316 stainless steel 593 and 649 C are continuing. Experiments similar to those previously performed on Type 316 stainless steel are being conducted on modified 9Cr-1Mo steel at 538 and 593 C. Four specimen configurations are being used: (1) low-cycle fatigue (LCF), (2) compact type (CT), (3) center-cracked tension (CCT), and (4) multiple-edge-notched tension (MENT) The LCF and MENT specimens have short (0.1 to 1.5 mm) cracks, and the CT and CCT specimens have long (25 to 35 mm) cracks. The range of the cyclic J integral has been shown to be a good parameter for characterizing fatigue-crack-growth rates when creep effects are negligible. The C* integral has been shown to be a good parameter for characterizing creep-crack-growth rates under static or slowly varying loading with steady-state creep across the remaining uncracked ligament. Transient effects during fatigue after a period of creep or vice versa can be interpreted in terms of the crack-tip-zone interaction model. Use of the MENT specimen configuration has been shown to provide a relatively simple and economic means of measuring creep-crack-growth at low propagation rates (near 1 mm per year) The general approach is being evaluated for cases where creep-fatigue damage may occur during dwell periods at some fraction (0 to 1.0) of the maximum cyclic load.

BRIGHAM YOUNG UNIVERSITY
Department of Chemical Engineering
Provo, UT 84602

05. MEASUREMENT AND PREDICTION OF LIQUID MIXTURE THERMAL CONDUCTIVITY AND VISCOSITY R. L. Rowley	$20,000	01-05 82-2

In spite of the importance of liquid mixture thermal conductivities and viscosities in energy technology, existing models and correlations are either inaccurate and inadequate or require multiple adjustable parameters for each specific system. This project has led to the development of a new predictive method for liquid mixture thermal conductivities and shear viscosities, based on the local composition concept for nonrandom liquid mixtures, which permits accurate estimation of these properties from thermodynamic data with no adjustable parameters. A high-precision capillary viscometer has been used to study a wide range of binary and ternary viscosities over a moderately wide temperature range at ambient pressure. These data have been used to test the newly developed model. Although the model contains only binary interaction terms obtained from equilibrium thermodynamic information, ternary as well as binary systems are accurately predicted by this method. Test system emphasis has been on highly nonideal mixtures containing polar and associating components. The temperature dependence of these mixture viscosities and the nature of aqueous systems are currently under investigation. Additionally, a new transient hot-wire thermal conductivity cell capable of making rapid and accurate liquid mixture thermal conductivity measurements has been designed. Construction of the apparatus is in progress. The local composition model has been used to make both binary and ternary mixture thermal conductivity predictions: while the binary results have been extremely accurate when compared to literature data, hardly any ternary mixture data have been found with which to compare the predictions. Experimental data obtained during the next year from the new thermal conductivity cell should remedy this situation.

BROWN UNIVERSITY
Division of Engineering
Providence, Rhode Island 02912

06. GEOMETRIC ANALYSIS OF THE ENSEMBLE OF SOLUTIONS IN TWO-PHASE FLOWS AND COMPLETE RESOLUTION OF THE PROBLEM OF CHOKING — $70,000 — 01-05 84-3

J. Kestin

The project studies a mathematical formalism for the qualitative analysis of the geometric-topological structure of all trajectories (solutions) of a two-phase model in a space formed with the state-velocity variables and physical distance. Such an analysis supplements the study of numerical solutions produced by an appropriate computer code. It serves to answer a number of questions of physics without actually solving the equations of the model, to establish a set of initial conditions for which the problem is well-posed, as well as that set for which no physically meaningful solutions exist. The most important advantage in carrying out such an analysis in detail is the fact that it provides us with a complete resolution of the problem of choking.

First, the analysis has shown that the commonly employed criterion $\Delta = 0$ constitutes merely a necessary condition for choking to occur, even though it also supplies us with an expression for the velocity of propagation of small-amplitude disturbances implied in a particular model. All points $\Delta = 0$ belong to one of two classes. Turning points are characterized by the fact that the sign of Δ changes along the trajectory. Such points correspond to choking at the end of the channel. By reverse integration it is possible to distinguish between physically possible and physically impossible inlet conditions. When certain additional conditions are satisfied, a point with $\Delta = 0$ becomes singular. There exists a variety of topological patterns generated by singular points. These may be classified according to the number k of trajectories which cross them. The patterns with $k > 2$ correspond to choking inside the channel. The formalism under study allows us to trace all trajectories (solutions) of this type, thus determining the inlet and exit conditions which induce and maintain choking, as well as the location of the choked cross-section.

An analysis of a general form of the system of equations which govern steady-state multiphase flows shows that the state-velocity which exists at a choked section is independent of the closure conditions (phenomenological assumptions), which, however, in the presence of appropriate inlet conditions, determine the location of the choked cross-section.

A method of determining the character of the singular points has been worked out.

BROWN UNIVERSITY
Division of Engineering
Providence, Rhode Island 02912

07. IMPROVEMENT IN THE DESIGN AND EXTENSION OF OPERATING RANGE OF VISCOMETERS AND THERMAL CONDUCTIVITY CELLS $80,000 01-05 80-4
J. Kestin

This project continues the development of measurement of two important transport properties, the viscosity and the thermal conductivity. Work is underway on the modification of existing instrumentation to extend the ranges of pressure and temperature and to make measurements at combined high temperatures and pressures (300-400 C and 30-40 MPa) while retaining the accuracy of 0.1-0.5% which is the state-of-the-art for more modest conditions. Working simultaneously in the same carefully staged way, the goal for thermal conductivity measurements is to develop instrumentation that will cover the range up to 50 MPa and 600°C. With each staged increase in capability, extensive measurements are being made on selected substances to secure results before the instruments are exposed to increased risk. New measurements on the viscosity of H_2O and D_2O were performed up to 200°C to create a basis for the search for a law of corresponding states. Preliminary calculations seem to point to the existence of such a law with appropriately chosen reference values. In the thermal conductivity instrument measurements on the mixtures of Ar-CH have been completed. The next step consists of a series of measurements on mixtures involving two gases of nearly identical molecular weight but different structure. Measurements on N_2-CO show that the mixtures have the same viscosity as N_2 or CO (both nearly equal), but significantly different thermal conductivity. This may prove of theoretical interest in statistical mechanics. The selected substances are chosen to make a contribution to the national energy program as well as to the development of methods of calculation for use in science and industry.

UNIVERSITY OF CALIFORNIA, DAVIS
Department of Mechanical Engineering
Davis, California 95616

08. STABILITY AND STABILIZATION OF PREMIXED FLAMES $53,000 01-03
84-2
C. K. Law

The program aims to investigate effects of heat loss, aerodynamic stretching, and preferential diffusion on the limits and mechanisms for the generation, suppression, and sustenance of flame-front corrugations; to identify the influence of these corrugations on flame stabilization; and to explore possibilities of widening the stabilization limits. Experiments are being conducted by using a variety of laboratory-scale burners to systematically isolate and identify the importance of various system parameters on the phenomena of interest. Theoretical analyses using large-activation-energy asymptotics are performed for the various experimental flame configurations to provide guidance and confirmation. During the reporting period an experimental investigation has been completed on an accurate determination of laminar flame speeds from stretched flames. In this project the effects of stretch on the determination of the laminar flame speed have been experimentally studied by using the positively-stretched stagnation flame and negatively-stretched Bunsen flame, and by using lean and rich mixtures of methane, propane, butane, and hydrogen with air whose effective Lewis numbers are either greater or less than unity. Results demonstrate that flame speed determination can be influenced by stretch through preferential diffusion and flow divergence. Recent data on flame speed including the present ones have been examined from the unified viewpoint of flame stretch, leading to satisfactory resolution of the discrepancies between them. The present study also proposes a methodology of determining the laminar flame speeds by using the stagnation flame and linearly extrapolating the data to zero stretch rate. An experimental study on the dynamics of polyhedral flames stabilized on a burner rim has also been initiated. Both the stationary and spinning modes of combustion have been identified and characterized, and effects due to heat loss to the rim have been quantified.

UNIVERSITY OF CALIFORNIA, LOS ANGELES
School of Engineering and Applied Science
Department of Mechanical, Aerospace and Nuclear Engineering
Los Angeles, California 90024

09. FLOW AND HEAT TRANSFER IN $66,000 01-02
UNIFORM AND NON-UNIFORM POROUS BEDS 82-3
Ivan Catton

The research covers two broad areas: 1) single-phase convection in porous media and 2) two-phase convection in porous media. The two areas of study are further sub-divided into a) forced convection, b) free convection, c) free/forced convection, d) fluidization under two-phase flow conditions and e) effects of bed non-uniformities. Layered porous media with intervening liquid regions as well as layers with no through flow will be part of the study. The objective of this research is to develop physical understanding of the governing phenomena and models for prediction of heat transfer by theoretical and experimental means.

An experimental investigation of the effect of media Prandtl numbers on heat transfer has been completed. Stainless steel, lead, and glass particles of various diameters were used with silicon oil, water and mercury to obtain empirical relationship between Nusselt number, Prandtl number, Rayleigh number and Kozeny-Carman Coefficient was developed that correlates all the data to within ± 10%.

A numerical study of cellular convection within an unstably heated homogeneous porous layer confined between two-isothermal horizontal boundaries is underway. A general non-Darcian motion equation was developed to investigate inertial effects and a single energy equation was used for the temperature field. Solutions of the thermohydrodynamic field were obtained with a mixed finite difference-spectral numerical scheme and closure was achieved using a thermodynamic criterion based on the Glansdorff-Prigogine stability criterion (wavenumber selection). The results compare satisfactorily with heat transfer measurements.

An apparatus has been constructed and tested to study multi-dimensional two-phase flow in porous media with phase change. Measurements and analysis will begin this fiscal year.

University of California, San Diego
Scripps Institution of Oceanography MC A-013
La Jolla, California 92093

10. Nonlinear Dynamics of Dissipative Systems $50,000 01-06
Henry D. I. Abarbanel 84-2

This research involves investigating the mechanisms which make for efficient energy transfer from a slow, mean motion to a system characterized by high frequencies relative to the mean motion. The basic mechanism of viscosity in a fluid is an example of this. The goal is to learn how to quantitatively characterize the "effective" or "eddy" viscosities used in phenomenological studies of energy, momentum, and other transfers of a turbulent fluid. The work is proceeding by studying analytically and numerically the behavior of systems of a few degrees of freedom as a function of their coupling.
The systems are known numerically and, in certain regimes using the Melnikov method, analytically to exhibit chaos. In regimes of parameter space where the motion is regular or laminar the energy transfers are weak; in regions of chaotic motion the rate of transfer can be given a quantitative interpretation in terms of phase space correlation functions. The exponential decay of these functions on a rapid time scale, possibly related to the nontrivial Liapunov exponents of the chaotic motion of the rapidly evolving system, gives an additional rapid rate scale for the transfer of energy to the coupled slow system. Applications to energy problems include all those setups where "friction" or dissipation of a slowly evolving flow are the result of its interaction with a higher frequency system.

UNIVERSITY OF CALIFORNIA, SANTA BARBARA
Department of Mechanical and Environmental Engineering
Santa Barbara, CA 93106

11. CONVECTION HEAT TRANSFER IN THE CRITICAL REGION OF FLUID MIXTURES. $40,000 01-02 83-2
E. Marschall

The purpose of this project is to determine convective heat transfer rates in the vicinity of the critical point of liquid mixtures. The ability of pure liquids at critical or slightly super critical conditions to allow very large heat fluxes to occur at very small temperature differences has been established. It is the basic goal of this study to determine whether or not the same phenomenon exists for liquid mixtures. To accomplish this goal, heat transfer rates near the critical point of liquid mixtures are being measured depending on mixture concentrations, temperature differences, and material of heating surface. Emphasis is also placed on the study of the influence of azeotropic behavior and retrograde evaporation or condensation on the heat transfer characteristics. The overall result expected from this work is a model for the prediction of heat transfer rates in the critical region of binary mixtures.

UNIVERSITY OF CHICAGO
Enrico Fermi Institute
Chicago, Illinois 60637

12. FUNDAMENTALS AND TECHNIQUES OF NONIMAGING OPTICS R. Winston, J. O Gallagher	$115,000	01-06 81-3

Nonimaging optics departs from the methods of traditional optical design to develop instead techniques for maximizing the collecting power of concentrating elements and systems. Designs which exceed the concentration attainable with focusing techniques by factors of four or more and approach the thermodynamic limit, are possible. This is accomplished by applying the concepts of Hamiltonian optics, phase space conservation, thermodynamic arguments and radiative transfer methods. Concentrators based on this approach are finding increasing use in solar energy and a variety of other applications, including the by now well known non-tracking Compound Parabolic Concentrator (CPC). To develop the underlying theory and design principles a theoretical formalism has been established based on a quantity called the geometric vector flux J, whose properties lead quickly to the discovery of new ideal concentrator solutions and an improved understanding of existing designs. Recently fundamental nonimaging optical principles have been extended to systems where physical optics effects play a role which has important consequences for concepts based on diffractive optics (e.g., holograms). A promising method for deriving the vector flux yield for particular concentrator geometries based on the introduction of a pseudopotential, has been identified. Present objectives of this basic research program are to extend the development of these concepts not only for solar energy applications but for more general problems involving the transmission and detection in other portions of the electromagnetic spectrum as well.

CLARKSON COLLEGE OF TECHNOLOGY
Department of Chemical Engineering
Potsdam, New York 13676

13.	BURSTING IN STEADY AND PULSATNG TURBULENT PIPE FLOW J. B. McLaughlin and R. J. Nunge	$75,000	01-02 82-3

The objectives of the research project are: (1) to gain an improved understanding of the production of turbulence in the viscous wall region of turbulent pipe flow; (2) to determine the effects of externally imposed pressure pulsations on turbulence structure and momentum, heat, and mass transfer in turbulent pipe flow; and (3) to determine the feasibility of exploiting such effects to increase the efficiency of heat exchangers and similar devices. A combination of computer modelling and laboratory experiments is being used to achieve these goals. The computer modelling involves the solution of a nonlinear, time-dependent model of the Navier-Stokes equation in which the axial and spanwise average of the axial component of velocity is set equal to a mixing length profile for all points lying outside the viscous wall region (which has a thickness roughly equal to 30 in wall variables) at each instant of time. In the case of steady turbulent flow, the model yields predictions for the intensities, production rate, and mean velocity profile which are in good agreement with experiment in the viscous wall region. In addition, detailed information about the structure and time dependence of the coherent eddies which dominate the production of turbulence in the viscous wall region has been obtained. The effect of pulsation on the behavior predicted by the model has been studied for a pulsation period equal to 100 in wall variables. It has been found that there is a large increase in the phase-dependent production of turbulence in the part of the cycle for which the bulk velocity is larger than average. Experiments are being carried out in order to check the predictions of the model about the effect of pulsations on momentum transfer and wall shear stress fluctuations.

COLORADO SCHOOL OF MINES
Department of Chemical Engineering
and Petroleum Refining
Golden, Colorado 80401

14. RADIATIVE HEAT TRANSFER IN OIL SHALE RETORTING Michael C. Jones	$ 0	01-02 81-2

Successful modeling of oil shale retorting and other fossil fuel conversion processes depends upon an accurate knowledge of the transport processes occurring. Among these are the transport of heat between combustion gases and rock particles and the axial transport of heat along the retort. At the temperatures of the combustion zone in a retort, the dominant mode of heat transport between combustion gases and solids is radiation. The objective of this project is to provide a basis for modeling by experimental measurements and by evaluation of models of the heat transfer processes. The experimental method is to observe the propagation down a packed bed of inlet gas temperature disturbances, and to infer interphase heat transfer coefficients and axial conductivities by comparison with the results of a differential equation model containing those parameters. The comparison may be made in time, Laplace, or frequency domains. The effect of gas radiation will be determined by performing the experiment with carbon dioxide rich mixtures and with non-radiating gas (nitrogen) as a control.

Frequency response experiments have been carried out on a 5" diameter packed bed of alumina spheres over a range of temperatures, flow rates and diameters. Measurements of both amplitude ratio and phase lag for thermometers at two different locations have allowed the testing of different models and the determination of model parameters. These measurements show good promise of allowing the separation of radiation and conduction effects.

COLORADO SCHOOL OF MINES
Department of Chemical Engineering
and Petroleum Refining
Golden, CO 80401

15. MEASUREMENT AND CORRELATION OF HEAT TRANSPORT PROPERTIES FOR MODEL COAL LIQUID COMPOUNDS USING AN EXISTING HOT WIRE INSTRUMENT $80,000 01-05
83-2
E. Dendy Sloan, Michael S. Graboski

The basic goal of this research is to determine some thermophysical properties of fluids encountered in the process of coal liquefaction. The research includes three major tasks. First, an expanded data base will be developed for coal liquids and model compounds. Second, these data will be tested against existing correlations for liquid thermal conductivity. Third, an instrument developed under a previous contract will be evaluated as a device for determining the thermal diffusivity of pertinent coal derived liquids.

CORNELL UNIVERSITY
Department of Electrical Engineering
Ithaca, New York 14853

16.	COMBUSTION CONTROL WITH SMART SENSORS G. L. Wolga	$80,000	01-03 82-3

The objective of this project is to develop a "smart" spectroscopic sensor suitable for monitoring gaseous combustion products by differential infrared absorption spectroscopy and to use the sensor to demonstrate closed loop combustion control of a two-burner furnace. The sensor is a computer controlled tunable acoustooptic infrared filter with sufficient resolution to resolve individual vibration-rotation absorption lines in the 5 - 6.5 micron spectral region. It will be self calibrating with respect to temperature changes and thus the sensor can operate unattended indefinitely. A tunable CO laser has been used to develop an accurate tuning curve for the filter in the 5 to 6.5 micron spectral region. Differential absorption measurements on CO and CO_2 in a heated cell are in progress to demonstrate the sensitivity of the filter, to select appropriate spectroscopic signatures, and to provide data for design of the self calibrating feature. Subsequently, infrared differential absorption spectroscopy will be carried out on combustion products from a flat flame burner; a turbulent, swirl burner; and finally, a two-burner furnace. This furnance will be fueled through control valves adjusted by a computer with the spectroscopic sensor providing quantitative information on combustion product concentrations sufficient to optimize furnance efficiency. Design and construction of the test burners is underway. Data analysis procedures for handling absorption integrated over a path length have been developed.

CORNELL UNIVERSITY
Department of Mechanical and Aerospace Engineering
Ithaca, New York 14853

17.	FUNDAMENTAL HIGH PRESSURE DROPLET COMBUSTION CHARACTERISTICS OF EMULSIONS AND MIXTURES C. T. Avedisian	$42,000	01-05 83-3

This work is designed to provide a fundamental understanding of the evaporation/combustion and internal boiling characteristics of droplets of mixtures and emulsions over a range of ambient pressures. For this purpose several experimental and analytical efforts are underway. Droplet combustion experiments are to be performed in a drop tower. In this technique, the combustion chamber, test droplet, and associated instrumentation are in free fall. Measurements planned include the effects of composition and ambient pressure on both the temporal variation of droplet diameter and vapor explosion intensity. This latter problem is also being studied in more detail in a second experiment designed to provide quantitative information on the specific mechanisms and parameters controlling the internal boiling characteristics of fuel droplets which are miscible mixtures of liquids. Light test droplets will be levitated, superheated, and made to vaporize in a flowing stream of another heavier immiscible field liquid in a vertical chamber, the pressure of which will be controlled up to 20 atm. Tasks completed and under development are the following: 1) a new and accurate method has been developed for predicting the liquid phase temperature required to initiate vapor explosions in multicomponent miscible liquids; 2) a model for bubble growth within superheated liquid droplets has been developed; 3) the droplet levitation experiment has been contructed and undergone initial testing and 4) the drop tower is being constructed.

ELECTROCHEMCAL TECHNOLOGY CORP.
3935 Leary Way, NW
Seattle, Washington 98107

18.	ELECTROCHEMICAL WEAR MECHANISM AND DEPOSIT FORMATION IN LUBRICATED SYSTEMS T. R. Beck	$66,000	01-01 82-3

The objective of this research is to measure and determine the importance of electrokinetic- or zeta- corrosion and deposit formation in lubricated rolling and sliding systems. Zeta corrosion is a phenomenon identified and modeled in 1968 for hydraulic servo control valves in commercial jet airplanes. This problem has now been solved by appropriate additives based on the theory. The approach of the present research is to compare measurements of wear for rolling and sliding lubricated systems to calculated zeta corrosion rates based on extensions of the valve wear model. The main challenge is distinguishing wear by zeta corrosion from abrasive and adhesive wear. In the first eight months of the contract required physical properties were measured for eight common lubricating oils and measurements were made of wall current density generated and size of wear scars. A good agreement was obtained between the measured wall current density and that predicted by the model for a simulated steel journal bearing. Wear on the plane polished journal turned out to be much greater than predicted by the measured and calculated wall current density based on the gross hydrodynamics. The wear scars consist of furrows with parallel scratches and furrows with micropits. With a Nylon cloth attached to the shaft wear scars are about the same size but virtually all pitted furrows. Zeta corrosion caused by passage of metal surface roughness or the roughness of the Nylon weave over the journal surface is indicated. Experiments to distinguish unambiguously zeta corrosion are underway.

FLOW INDUSTRIES, INC.
21414 68th Avenue South
Kent, Washington 98032

19. DIRECT NUMERICAL SIMULATIONS OF $60,000 01-02
TURBULENT HEAT TRANSFER 84-3
Ralph Metcalfe

The purpose of this research is to apply the technique of direct numerical simulation to the study of turbulent heat transfer. Direct numerical simulation techniques have been applied successfully to such problems as the testing of turbulence theories, an examination of second order closure modeling assumptions, and addressing questions about the basic physics of turbulent diffusion, mixing layer control through forcing, homogeneous turbulence decay and the decay of turbulence in the presence of background stratification. There are some significant advantages to this approach. Since the flow field is known in detail at each time step, quantities which are difficult or impossible to measure in the laboratory can be computed. No closure modeling is done, so that no ad-hoc assumptions are introduced. The initial and boundary conditions as well as other critical parameters can be precisely controlled, permitting a systematic study of their effects on the evolution of the flow field.

The objectives of the proposed work are to make use of the direct numerical simulations to develop a better understanding of the effects of turbulence on heat transfer and to improve existing turbulence models. The application of spectral numerical methods to problems of this type will be studied so that these techniques will be of increasing practical utility in the future. A series of problems of increasing complexity will be simulated, beginning with Couette flow. The work will focus on the effects of large scale structures and shear on the flow field.

GENERAL ATOMIC COMPANY
10955 John Jay Hopkins Drive
San Diego, California 92121

20. FLUID MECHANICS OF ACOUSTIC RESONANCE IN HEAT EXCHANGER TUBE BUNDLES $10,000 01-02
82-3
R. D. Blevins

The purpose of this study is to develop a predictive fluid mechanic model for acoustic resonance in shell and tube heat exchangers. Acoustic resonance in heat exchangers is the result of acoustic oscillations of gas in sympathy with periodic fluctuations in the flow over tubes. In the experimental phase of the program, a simulated tube bundle is being constructed which will be tested in air flow. Direct measurements of the onset of resonance, intensity and mode of acoustic pressure will made with microphones, and measurements of the exciting fluid dynamic fluctuations about the tube will be made with hot wire anemometers. The results will be processed on-line using fast Fourier transforms. In the theoretical phase of the program, a linear acoustic model for the phenomenon will be developed using acoustic source and dissipation terms and a calculated acoustic mode shape. The experimental results will then be used to refine the acoustic source and dissipation terms, develop a fundamental understanding of the fluid dynamic and acoustic interaction. A nonlinear model for the self excitation will then be developed using Lighthill's formulation for aerodynamic sound in interaction with the coherent structures in the flow due to vortex shedding from the tubes.

GEO-CHEM RESEARCH ASSOCIATES
400 East Third Street
Bloomington, Indiana 47401

21. PREDICTIVE MODELING OF URANIUM ROLL TYPE DEPOSITS — $109,000 — 01-06 83-3
P. J. Ortoleva

Oxidizing meteoric waters percolating through a reduced sandstone aquifer can cause the accumulation of uranium and other ores at the redox interface. The oxidation of pyrite to hemtite or goethite can lead to several instabilities underlying observed ore body properties. The existence (and in some cases non-uniqueness) of propagating redox fronts in ore-reductant systems (such as pyrite) was demonstrated and a general exact value for its speed was obtained for the lossless aquifer. The nonexistence of constant velocity redox fronts in multireductant systems was proven analytically and shown numerically to correspond to an accumulation of one mineral at the front of the other - the essential trapping process leading to redox deposits.

A class of instabilities was found when reaction-induced porosity variations were allowed to interact with the percolation flow through the porosity-dependent permeability of Darcy's law. The planar front of dissolution of soluble components in a sandstone aquifer (as pyrite in oxidizing inflow waters) was found analytically to be unstable to the formation of bumps. The range of wavelengths of the most rapidly growing array of bumps brackets the observed wavelengths in roll front deposits when geologically reasonable flow and porosity values were used in our expressions. Numerical simulations of the full nonlinear problem confirmed the linear analysis, and showed that, interestingly, a single bump (in the shape of the surface on which porosity changes) can branch into two fingers. Even very small changes in porosity across the redox front can lead to this fingering.

Nonlinear transport/reaction interactions underly the genesis of uranium roll-front deposits and directly control their geometry and quality. These insights are potentially very useful for exploration.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Science Division
Idaho Falls, Idaho 84315

22. CRACK CHARACTERIZATION WITH ULTRASONIC NDE — $110,000 — 01-03 83-3

D. D. Keiser, J. A. Seydel
B. A. Barna, J. A. Johnson
D. M. Tow

The purpose of this research is to develop the instrumentation and analytical models that can predict and identify the frequency dependence of the amplitude and phase of ultrasonic echoes from defects. The approach treats the transducer/media/defect combination as a linear system which allows separation of the individual contributions to the signal detected at the transducer. A model based on the numerical solution of the partial differential wave equations has been developed to provide "snapshots" of the transducer field both before and after it has interacted with the flaw. This information is then compared to experimental data collected at a large number of transducer positions. Since the objective is to characterize defects, a number of techniques are being developed to display frequency-domain information which relates to the type of defect. One method is to display the phase and amplitude spectra values as a function of frequency and transducer position.

IDAHO NATIONAL ENGINEERING LABORATORY
Materials Technology Division
Idaho Falls, Idaho 83415

23. ENGINEERING ANALYSIS OF ELASTIC-PLASTIC FRACTURE $165,000 01-04
81-4
W. G. Reuter

The objective is to improve design and analytical techniques for predicting the integrity of flawed structural components. The research is primarily experimental, with analytical evaluation guiding the direction of experimental testing. Tests are being conducted on a material (a modified ASTM A-710) exhibiting a range of fracture toughness but essentially constant yield and ultimate tensile strength. As test temperture increases, the specimen configuration-fracture toughness relationship compiles initially with requirements for linear elastic-fracture mechanics and extends beyond the range of a J-controlled field. Presently, compact tension (3-point bend specimens will also be used in the future) are being used to develop state-of-the-art fracture mechanics data on the lower shelf (K_{Ic}), transition zone (J_{Ic}, J-R curves, etc.), and on the upper shelf (J_{Ic}, J-R curves, etc.). Results from the lower shelf and transition region are being used to predict failure conditions for specimens containing surface flaws. Predictions are then compared with experimental test data. These comparisons are presently underway for 6.4 and 12.7 mm thick surface-flawed specimens. Metallographic techniques are being used to measure crack tip opening displacement for comparison with analytical models. Laser interferometry and infrared thermography techniques will be used to evaluate and quantify the deformation in the crack region.

ILLINOIS INSTITUTE OF TECHNOLOGY
Department of Electrical Engineering and
Department of Chemical Engineering
Chicago, Illinois 60616

24. METHOD OF VIBRATIONAL CONTROL IN THE PROBLEM STABILIZATION OF CHEMICAL REACTORS $70,000 01-03 84-3
S. M. Meerkov and A. Cinar

The objective of this research is to develop the vibrational control technique for complex nonlinear dynamic systems with multiple steady states and limit cycles. From the mathematical standpoint, the goal of the project is to analyze the effects of fast parametric oscillations on the dynamics of the system. The two main objectives of the first period of the project have been formulated as:

(1) experimental study of vibrational control of a CSTR with homogeneous liquid phase reaction,

(2) development of the theory of vibrational control for nonlinear systems with multiple (nonzero) steady states.

These objectives have been achieved, and the following results, pertaining to objective 1 and 2, have been obtained:

1i. A theoretical and numerical investigation of the chosen reaction system (the second order exothermic reaction between $Na_2S_2O_3$ and H^2O^2 in aqueous solution) have been conducted.

1ii. An experimental study of the vibrationally controlled plant unit with the chosen reaction system has been undertaken. The experimental results are in good agreement with theoretical predictions: (a) the vibrationally controlled CSTR has a stable periodic regime near an unstable steady state of the stationary CSTR system; (b) the vibrationally controlled CSTR has an increased average conversion in comparison to that of the stationary CSTR with the same residence time; (c) the average steady state characteristics of the vibrationally controlled CSTR have smaller negative slope parts compared to those of the stationary CSTR. Additional experiments are being conducted to further quantify these results.

2i. Conditions of vibrational stabilizability of nonlinear systems with multiple (nonzero) steady states have been found;

2ii. Conditions of vibrational controllability for nonlinear systems have been formulated;

2iii. The transient behavior of vibrationally controlled nonlinear systems has been analyzed.

ILLINOIS INSTITUTE OF TECHNOLOGY
Department of Mechanical and Aerospace Engineering
Chicago, Illinois 60616

25. INTERFEROMETRIC MEASUREMENTS IN DOUBLE-DIFFUSIVE SYSTEMS $50,000 01-03
84-3
William M. Worek
Zalman Lavan

The objective of the project is to develop an experimental technique to measure two scalar variables in double-diffusive or other two component systems. The two frequency optical decomposition technique uses a dual frequency Mach-Zehnder Interferometer to simultaneously determine the local gradients of two scalar variables in the test system. Interferograms taken at the two different frequencies are analyzed using index of refraction data which is a function of temperature and concentration. The experimental program will be integrated with an analytical approach in an attempt to identify and assess the potential application of such a technique and the impact on stability studies in double-diffusive systems. Currently, preliminary experiments are being performed to assess the potential of the technique using a narrow frequency range. Also, a test system has been constructed to acquire index of refraction data of salt-water solutions, with an accuracy of 10^{-7}, at different concentrations and temperature for wavelengths typical to laser sources. This data, which is not available in the literature, will enable the proper selection of the two wavelengths used in system so as to maximize the resolution of the two scalar variables.

UNIVERSITY OF ILLINOIS
Department of Civil Engineering,
Mechanics, and Metallurgy
Chicago, Illinois 606800

26. CONTINUOUS DAMAGE THEORY $41,000 01-04
Dusan Krajcinovic 83-3

The study centers on the phenomenological description of the nucleation and growth of microdefects in a metallic solid and their influence on the mechanical response. The analytical work will proceed within the scope of the Continuous Damage Mechanics, according to which the distribution and density of microdefects can be represented by a set of appropriately selected internal variables.

Present investigations focus on the basic aspects and definitions to prepare the groundwork and reconcile several different models. It was, for example, found that in case of a general microcrack field a distinction must be made between the microcrack distribution and the damage consistent representation of a field of flat microcracks. The projection of these vectors on a plane through the observed point is a physically reasonable measure of damage.

Subsequently the focus will shift on the investigation of the interaction of viscous effects (reflecting the boundary slip) and the brittle effects (growth of microcracks). The established continuum model will be used to study problems such as creep rupture, fatigue, etc.

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, CA 91109

27. BASIC DATA FOR THE DEVELOPMENT OF MOLECULES AS THRESHOLD ELECTRON DETECTORS $68,000 01-03 82-3

A. Chutjian, S. Alajajian

Measurements and calculations are being made of, at high electron energy resolution, lineshapes and cross sections for attachment of thermal electrons to a number of electron-attaching gases. Perfluorinated carbon and chlorofluorocarbon compounds have been shown to be viable candidates for use a molecular detectors for extremely low-energy (0-50 millielectron volt) electrons. The use of such detectors has been demonstrated in our own laboratory in obtaining the first threshold photoelectron spectra of N_2, CO and O_2 using SF_6 and CFCl3 as detectors. It is desired to study the use of other gases, as well as temperature effects, to obtain the narrowest bandwidth for zero-energy electron detection. Under the present grant we have observed extremely narrow (slit-width limited) structure at threshold which arises from the s-wave divergence of the attachment cross section $\sigma_A (\varepsilon) \sim \varepsilon^{-1/2}$ electron energy $\varepsilon \rightarrow 0$. We have clearly observed this structure in eight molecules thus far. Further studies of this phenomenon are continuing. We have also reduced to practice a new type of source for generating negative ions based on these large attachment cross sections. Extension of this source in terms of ionic species generated, and current densities possible, is planned.

JET PROPULSION LABORATORY
California Institute of Technology
Pasadena, CA 91109

28. THIN FILM CHEMICAL SENSORS $110,000 01-03
BASED ON ELECTRON TUNNELING 83-4
J. Lambe, S.K. Khanna

The objective of this three year program is to understand the physical mechanism of detection underlying a totally new chemical detection concept which utilizes electron tunneling as the sensing mechanism. The technical approach involves investigations of the tunneling spectrum (second derivative of current with respect to voltage versus voltage) of metal-metal oxide-metal (e.g., aluminum-aluminum oxide-gold) tunnel junctions which are exposed to chemicals such as halogens. Some of the other key questions to be addressed in this project are: 1) what are the ultimate sensitivity and selectivity, and 2) what are the contributions of the insulating layer and the top porous metal electrode. These electrical measurements, in addition to surface and interface studies, should help us to understand the detection mechanism. A successful program can pave the way for the development of a compact thin film electronic chemical sensor for use in the automation of the chemical processes, and hence, to increase reliability and productivity. Al-Al_2O_3-Au (MIM) tunnel junctions were fabricated using an oil-free ultra-high vacuum system. The iodine signal was observed by measuring the tunneling spectrum of the MIM tunnel junction exposed to iodine. We have observed the intrinsic surface state on gold surface using electron tunneling spectroscopy. These surface states have been identified as playing a key role in the chemical detection mechanism. We have detected iodine in hexane solution down to parts per billion. We have also detected mercury vapor, bismuth metal and ethylene dibromide (EDB) using this technique.

LAWRENCE BERKELEY LABORATORY
Energy and Environment Division
University of California
Berkeley, CA 94720

29. CONTROLLED COMBUSTION A. K. Oppenheim	$180,000	01-05 79-6

The principal objective of this study is the acquisition of fundamental knowledge required for the development of controlled combustion systems. Such systems offer the prospect of maximizing thermal energy conversion efficiency, minimizing pollutant emissions, and optimizing the tolerance to a wide variety of fuels. A thorough understanding of ignition--the initiation of a self-sustained exothermic process of combustion--is for this purpose of essential importance. The major objective of the experimental program is the establishment of a fundamental background for the design of enhanced ignition systems. Of prime significance in this respect is the determination of the role of active radicals. This is accomplished by the use of a high frequency response molecular beam mass spectrometer that has been designed and built especially for this purpose. The corresponding theoretical approach is based on an extended thermo-chemical analysis for auto-ignition in a closed system, following the method of approach developed by Semenov and Frank-Kamenetskii. This is supplemented by numerical modeling of jets and flame propagation in turbulent flow. So far we have succeeded in measuring concentration histories of major chemical species, temperature, and pressure at a 100 microsecond time resolution in the course of a transient combustion process initiated by flash photolysis in a methane/oxygen/nitric dioxide/argon mixture. In the concomitant analytical studies we have been able to deduce the classical first, second, and third auto-ignition limits for the oxidation of hydrogen on the basis of comprehensive thermo-chemical computations, and to model the formation and inflammation of a turbulent jet. Future plans include measurement of temperatures and species concentration histories in a pulse plasma jet, and the development of a corresponding thermo-chemical analysis of the process.

LAWRENCE BERKELEY LABORATORY
Physics Division and
Accelerator and Fusion Division
University of california
Berkeley, California 94720

30. STUDIES IN NONLINEAR DYNAMICS $100,000 01-06
Allan N. Kaufman, Robert G. Littlejohn 80-3

This project involves studies of fundamental properties of nonlinear dynamical systems which arise in physical situations of importance to energy research. Four main subjects are being explored. First, theoretical studies to generalize the WKB representation of wave phenomena are in progress. In this work, caustics are avoided by working in ray phase space. The Maslov concept is generalized by utilizing Heisenberg and metaplectic operators to represent phase space translations and rotations. In this way, WKB eigenfunctions are obtained in symplectically covariant form, exhibiting no caustic singularities. Second, modern Hamilionian concepts are applied to deal with classical perturbation theories, in particular averaging methods based on slow and fast space-time scales. Reduction techniques yield systematic Hamiltonization of many models in current use, e.g., guiding-center motion and wave modulation. Third, action principles are being used to imbed single-particle Lie-transform perturbation methods in collective models, such as Vlasov-Maxwell systems. Nonlinear phenomena (e.g., ponderomotive forces) are thus dealt with self-consistently. Fourth, a new formulation of conservative dissipative processes is being explored, in which the entropy and energy functionals jointly generate the time-evolution of the system.

LAWRENCE LIVERMORE NATIONAL LABORATORY
Engineering Division
P. O. Box 808
Livermore, PA 94550

31. PROCESSING AND CHARACTERIZATION OF SCATTERED SIGNALS FROM ACOUSTIC TARGETS $160,000 01-03
82-4
B. Maxfield, E. Miller

We have begun in FY 1982 a study to develop a fundamental understanding of acoustic scattering from targets having relevance to material strength, for example flaws in metal components and welding faults, and to process such target signatures for possible automatic material characterization in non-destructive evaluation (NDE). This work is related to instrumentation development for NDE and more specifically with electromagnetic/acoustic scattering, and signal processing research. LLNL is currently involved in both areas using internal funds (engineering research) as well as reimbursable support (from various DOD agencies, and NRC).

LOS ALAMOS NATIONAL LABORATORY
Electronics Division
Los Alamos, New Mexico 87545

32. DEVELOPMENT OF THERMIONIC INTEGRATED CIRCUITS (TICs) $175,000 01-03
82-3
B. McCormick, D. Wilde, M. MacRoberts
D. Lynn, R. Dooley

The object of this project is to develop electronics that are capable of operating in both high-temperature and high-radiation environments while maintaining levels of circuit sophistication, integration, and reliability demanded of modern electronics. The approach taken for these active electronic-gain devices has been to use the intrinsically high-temperature phenomenon of thermionic emission in conjunction with the thin-film technology of integrated circuits to produce microminiature vacuum triodes. High-temperature tests have been conducted at 500 degree C for approximately 13,000 hours with no degradation in device characteristics. Devices have been subjected to total radiation doses of 10^{17} neutrons/cm^2 and 2.5 x 10^8 Rad(Si) gamma and to dose rates of 1.4 x 10^{16} neutrons/cm^2/s, 4.5 x 10^{10} Rad(Si)/s gamma and 2 x 10^8 Rad(Si)/s protons with no damage. An analysis of the frequency characteristics indicates that devices with gain bandwidth products of the order of 100 MHz can be designed with current technology. The level of integration for current technology is projected to be 1000 devices/in^2, which corresponds to medium scale integration. In addition, total heater power with and without reflective shielding has been analyzed and the results confirmed experimentally. These results show that for 1000 devices/in^2 with multiple subtrates in a package, the heater power will be 2.5 mW per device.

UNIVERSITY OF MARYLAND
Department of Electrical Engineering
College Park, Maryland 20742

33. STUDY OF MAGNETOSTATIC PROBLEMS IN NONLINEAR MEDIA WITH HYSTERESIS $[illegible]0,000 01-06 83-4
I. C. Mayergoyz

This project has two main research objectives: (1) to develop boundary Galerkin's approach and its quasi-finite-element realization in order to circumvent the difficulties which are related to the unbounded regions of field distribution, and (2) to investigate mathematical models of hysteresis and develop the methods for the calculation of magnetostatic problems in media with hysteresis.

As far as the first objective is concerned, the calculation of magnetic fields in unbounded regions will be reduced to coupled boundary/volume Galerkin's forms and a new quasi-finite-element projection technique wil be developed on this basis. The problems concerning convergence of the quasi-finite-element methods, existence and uniqueness of the solution of simultaneous nonlinear quasi-finite-element equations and global iterative methods of the calculation of the solution of these equations will be the focus of this research.

For the second objective, mathematical models of hysteresis as continuous superposition of rectangular hysteresis nonlinearities will be investigated. Special attention will be paid to the solution of identification problems and to the generalization of these models for the case of vector hysteresis. The application of continuation methods to the calculation of magnetostatic fields in media with hysteresis will be studied.

UNIVERSITY OF MASSACHUSETTS
Chemical Engineering Department
Goessmann Laboratory
Amherst, MA 01003-0011

34. A HIERARCHICAL PROCEDURE FOR FLOWSHEET, CONTROL SYSTEM, AND RETROFIT DESIGN FOR CHEMICAL PROCESSES $70,000 01-03
J. M. Douglas, M. F. Malone

New short-cut models for the energy integration of distillation sequences show that the total entropy of separation can be used to select the best sequence. A computer code based on this procedure runs essentially instantaneously, so that the use of heuristics for selecting distillation sequences can be avoided. Current efforts are to include complex columns, multiple feeds and sloppy spits into the code.

The new separation system selection procedure is also being incorporated into the "Expert System" for developing base-case designs and evaluating process alternatives. In addition, the "Expert System" is being modified so that it will run "instantaneously." Moreover, systematic procedures for the retrofitting and steady state control of complete plants, which will serve as the knowledge base for "Expert Systems" have been developed and are being tested.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, Massachusetts 02139

35. TURBULENT PREMIXED FLAME STUDY $140,000 01-05
83-3
Wai Cheng, James Keck
Steve Pope (Cornell University)

This program is a combined experimental and theoretical study of premixed turbulent flames. The primary aim of the experiment is to study the gross behavior and some detailed properties of statistically spherical flames over a very wide range of operating conditions. It is emphasized that the range of operating conditions is sufficiently wide to encompass qualitatively different regimes of combustion. The theoretical part of the program centers on calculations of the joint probability density function (pdf) of the velocity and species concentrations. This approach - to solve a transport equation of the joint pdf - avoids the closure problem normally associated with turbulent velocity fluctuations and non-linear reaction rates. In both the experimental and the theoretical effort, the primary variables being examined, for a flame of a given geometry and fuel/air ratio are a Reynolds number based on the turbulent strain rate, and a Damkohler number based on the ratio of the eddy time to the chemical reaction time. The development of flame balls under different turbulent conditions and stoichiometric ratios were recorded by high speed schlieren movies. The flame propagation characteristics were interpreted in terms of the turbulence structures measured with hot wire anemometry. In the theoretical study, preliminary calculations relating the normalized flame speed to the Damkohler number using the pdf formulation has been attempted. A "variable weighted" algorithm to treat the density difference between the burned and unburned mixture has been developed. The technique was applied to the calculation of a spherical flame.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
The Energy Laboratory
Cambridge, Massachusetts 02139

36. PISTON RING FRICTION AND VEHICLE FUEL ECONOMY 80,000 01-01 80-6
D. P. Hoult, J. M. Rife

The purpose of this research is to study the friction mechanism in automotive engines, in particular the components of frictional losses which arises due to the interaction bevween the piston rings and the piston liner. It is believed that this is the largest single component of friction in a typical automotive engine. The research underway comprises modelling and measuring the motion of each degree of freedom model of piston ring as it moves up and down in the piston groove has been completed and modifications necessary for the theory have been described. The next steps of this project, which are underway, are to study the ring twist and radial motion of rings in a experimental lubrication engine. The theory has suggested a novel concept for a gas lubricated ring which may greatly reduce engine friction.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Laboratory for Manufacturing and Productivity
Cambridge, Massachusetts 02139

37. A STUDY OF REDUCED ORDER MODEL REFERENCE CONTROL SYSTEMS FOR IMPROVED PROCESS CONTROL David E. Hardt	$54,000	01-03 82-3

The objective of this research is to provide a method for easy design of control systems when the plant involved is highly variable in both structure and parameter values. This typifies many manufacturing processes, which in general are highly sensitive to intrinsic properties of the infeed material, have poorly understood or controlled boundary conditions, and often have highly non-linear characteristics. In addition, the disturbances most frequent in a manufacturing process are best characterized as parameter changes rather than state variable changes. The choice of a parameter adaptive control paradigm is obvious since it has the property of optimizing system response characteristics in the face of wide plant parameter variations. Model Reference Adaptive Systems enjoy an ease of design and performance specification, and again seem applicable; however, there is a restriction within current theory that the plant be characterized in its structure well enough to have a reference model of identical order. This restriction implies a static plant structure and more _a priori_ knowledge than is often present.

Our research efforts so far have resulted in a unification of existing model reference adaptive control (MRAC) techniques with respect to their structure and design methodology. Through this we have identified the ability of each to deal with: 1) reduced order reference models, 2) noisy measurements, 3) disturbances, 4) sinusoidal learning signals, and large reference-input dynamic-range.

We found no single algorithm that gives acceptable performance, but through the techniques employed in our analysis, certain modifications were devised to improve the reduced order model, noise and reference input range problem.

Our next effort will involve more detailed evaluation of these findings using certain specific process models. The latter will be chosen on the basis of to their ability to truly test the MRAC effectiveness and according to the availability hardness for limited experimentation.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Laboratory for Manufacturing and Productivity
Cambridge, Massachusettts 02139

38. IMPROVEMENT OF RELIABILITY OF WELDING BY IN-PROCESS SENSING AND CONTROL 170,000 01-03 79-6
Koichi Masubuchi, Henry M. Paynter,
David E. Hardt, William C. Unkel

Over the years, the cost of constructing critical welded structures has increased drastically. A significant portion of the increase comes from required inspection and repair, while the direct cost of welding has increased only slightly. Closed-loop control of the welding variables represents promising cost-effective approach to improving weld quality and therefore reducing the total cost of producing welded structures.

This research program includes the following tasks:

(1) Demonstration of the measurement of weld size using mechanical impedance as a sensing technique for one of the two weld geometry measurements,
(2) Demonstration of a single variable control system using the above measurement,
(3) Demonstration of the ability to gain independent control of two weld geometry measures as described, for example, by the front and back bead widths of the weld metal,
(4) Demonstration of closed-loop geometry control with these two control variables,
(5) Expand the variables to be controlled from two geometry measures to include temperature history of the weldment,
(6) Implement the geometry control system on a mechanized welding system, and
(7) Provide one formal framework for implementation of welding control.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Department of Nuclear Engineering
Cambridge, Massachusetts 02139

39.	HYDRODYNAMIC PREDICTION OF MULTIDIMENSIONAL SINGLE- AND TWO-PHASE FLOW IN ROD ARRAY N. E. Todreas J. T. Robinson	$30,000	01-02 82-3

The objective of this research is to develop basic constitutive laws for the hydrodynamics of flow oblique to rod arrays. A thorough knowledge of the flow field within heat exchanging components comprised of rod arrays (i.e., heat exchangers, steam generators, nuclear reactor cores, condensers) is of primary importance to maintaining a high component efficiency, lifetime, and operational performance. Much thermal-hydraulic design and operational performance analysis of these energy components are being performed with discretized computer models. The recent advancements in high-speed digital computers and numerical computational methods have facilitated the expansion of these thermal-hydraulic codes from one- to two- and three-dimensional multiphase flow analysis. These new codes require as input constitutive laws of multidimensional, single- and two-phase flow fields within rod arrays such as those being developed in this project. Specifically, constitutive relations for single-phase flow resistance, two-phase flow resistance, and relative phasic motion (slip) will be developed based on measurements using atmospheric air/water within vertical test sections comprised of rod arrays inclined at 0, 30, 45, and 90 degrees to the direction of flow. Major tasks completed to date include (1) an evaluation of multidimensional flow resistance models for single phase turbulent flow, and (2) formulation of a model for relative phasic motion for bubbly flows.

UNIVERSITY OF MICHIGAN
Department of Mechanical Engineering and Applied Mechanics
Ann Arbor, Michigan 48109

40. LOSS CHARACTERISTICS OF CORD-RUBBER COMPOSITES $60,000 01-01
S. K. Clark 83-2

The research to be carried out under this contract is divided roughly into two phases. The first is completion of data acquisition on the loss characteristics of cord-rubber composites under both uniaxial and multiaxial stress states. This effort will utilize information currently available as well as measurements made here. The effects of prestrain, frequency, strain amplitude and temperature will be included in the assessment of the viscoelastic properties of these materials.

The major activity during the latter part of the work will be analysis and measurement of the rolling loss of a relatively simple pneumatic tire. The tire geometry will be essentially cylindrical in form, similar to the type of tire used in vehicles transversing soft or marshy terrain. These are essentially cylindrical rollers, but with end closures making it possible to inflate them. Analysis will be carried out using the viscoelastic material properties previously obtained, as well as finite element codes suitable for this type of problem. Comparison of calculated and measured rolling resistance values will give valuable insight into the types of finite element models best suited for this computation, and should give confidence to the tire industry in its efforts to apply finite element techniques to the calculation of tire operating properties.

Since tire rolling resistance represents a major component in the vehicular fuel consumption, minimization of it represents an important part of the overall national energy consumption effort.

UNIVERSITY OF MINNESOTA
Department of Mechanical Engineering
Minneapolis, Minnesota 55455

41. FLOW AND HEAT TRANSFER WITH IMPINGENG JETS AND WALL JETS — 88,000 — 01-02 81-6
R.J. Goldstein

This project is directed toward providing information on the flow, characteristics of impinging jets and wall jets and related problems in separated flows. Measurements of the heat transfer in the region of impingement are obtained for single jets entering a still ambient, for jets entering a crossflow, and for various one and two-dimensional arrays of jets. In addition to quantitative heat transfer measurements for these flows, visualization techniques are used to provide insight into the mechanism of the interaction of the jets and the local wall stress. A laser-Doppler anemometer was developed to provide detailed measurements of velocity distributions, velocity fluctuations, and Reynolds stresses in a plane wall jet. Such measurements should provide precision data for testing the validity of turbulent transport models that have been suggested. Considerable data have been obtained with a single jet; the results of several series of tests have been correlated with equations for both the peak heat transfer coefficient and the average heat transfer coefficient over various regions from the center of impingement. Also, data have been taken for a two-dimensional array of small jets impinging on a heat transfer surface; during these studies, a liquid crystal system was developed for studying the features of single and multiple jet impingement on a flat surface. The liquid crystal technique and study of the pressure distribution near individual jets on an impinging jet plate are being applied to inclined impinging jets. Related experiments on separated flows including the characteristics of horseshoe vortices are conducted using a mass transfer analogy.

NATIONAL BUREAU OF STANDARDS
Office of Standard Reference Data
Washington, D.C. 20234

42.	SUPPORT OF CRITICAL DATA COMPILATIONS David R. Lide, Jr.	$450,000	01-05 80-6

The Office of Standard Reference Data administers a collaborative interagency program for preparation of compilations of physical and chemical reference data. Each project supported is expected to lead to a publishable data compilation containing recommended values and accuracy estimates for the data set in question. Projects funded during fiscal year 1984 include work on photochemistry of transition metal coordination complexes; soft x-ray interactions with matter; properties of aqueous electrolytes at high temperatures; atomic transition probabilities of highly ionized atoms; thermodynamic tables for hydrocarbon isomer groups; ESCA data; ceramics phase diagrams; and alloy phase diagrams for systems of iron, alkali metals, actinide elements, and rare earths.

This project is included in the BES ENGINEERING RESEARCH program for administrative convenience. Coordination with NBS is accomplished in collaboration with several BES programs. BES FY 1984 funds for the project were provided by the Chemical Sciences and Materials Sciences divisions, and the Division of Engineering and Geosciences.

NATIONAL BUREAU OF STANDARDS
Thermophysics Division
Gaithersburg, MD 20899

43. THERMOPHYSICAL PROPERTIES OF $350,000 01-03
HYDROCARBON MIXTURES 84-3
H. J. Raveche, N. Olien

This project aims at the development of accurate measurement capabilities for the thermophysical properties of complex, multiphase, fluid mixtures containing hydrocarbons. The research is being done jointly by the Chemical Engineering Science Division at the NBS-Boulder facility and the Thermophysics Division at NBS-Gaithersburg, both within the NBS Center for Chemical Engineering. The properties involved are PVT (pressure-volume-temperature), phase equilibria (liquid-vapor and liquid-liquid equilibria) and transport properties (viscosity and thermal conductivity). The apparatus will be designed for use in corrosive, highly corrosive, and sometimes toxic and flammable fluids with measurements extending to high temperatures (900 K) and high pressures (30 MPa and in some cases 70 MPa). Current work involves: 1) construction of a constant-flow phase equilibria apparatus covering the range 300-800K with pressures to 30 MPa or more (construction completed; first test data taken); 2) construction of a multicomponent-multiphase nonsampling cell and a multicomponent two-phase cell with sampling valve for temperatures to 470K and pressures to 10 MPa (construction completed; tests being performed); 3) design and construction of new phase equilibria apparatus to cover the range 250-350K with pressures to 20 MPa (apparatus completed and operational), 4) automation of a Burnett PVT apparatus for the range 270-470 K (apparatus operational, automation progressing); 5) construction of a magnetic balance densimeter for the range 270-470 K with pressures to 15 MPa (in testing stage); 6) design of a torsional crystal viscometer for the range 300-750 K with pressures to 50 MPa or more (construction underway and all major design problems solved); 7) initiate design of high temperature thermal conductivity apparatus, 8) construction of a supercritical gas chromatograph for thermophysical property (e.g. diffusion coefficient) measurement in the supercritical region for the range of 300-400 K, 30 MPa, 9) design and construction of a film balance for measuring phase behavior of surfactant surface films.

Future work will include completion of the apparatus, performance testing, and the start of measurements on systems relating to long-term energy needs. In addition, other measurement techniques will be explored such as acoustic properties, light scattering, etc.

National Bureau of Standards
Tribology Group
Center for Materials Science
Gaithersburg, MD 20899

44. A STUDY OF THE CHEMICAL MECHANISM IN LUBRICATION $50,000 01-01
S. M. Hsu 84-4

Chemical mechanisms in concentrated contacts under lubricated conditions are largely not understood. This project will study systematically the nature and the extent of influence of chemical reactions in the contact zone on friction and wear. Surface topography of worn surfaces will be characterized to predict oil film thickness under different speed, load ranges in a NBS developed four-ball wear tester. Micro-asperity temperatures and the wear film temperatures of the oil film will be calculated using Archard-Jaeger equations as well as finite-element analysis techniques. Pure model structures will be used as lubricants to test the effects of chemical functional groups on friction and wear. Chemical kinetic studies on tribochemical reaction rate constants for various classes of compounds under wearing conditions will be compiled. A theoretical model linking elastohydrodynamic theories to tribochemical rate constants with materials properties will be attempted to predict lubrication effectiveness a priori.

CITY UNIVERSITY OF NEW YORK
The City College
Department of Chemical Engineering
New York, NY 10031

45. TOPICS IN PHYSICO-CHEMICAL HYDRODYNAMICS $250,000 01-06 80-8
Benjamin G. Levich

This research comprises two main directions:

(i) Fully Developed Turbulence (FDT). We aim at the entirely novel understanding of the nature of FDT. We assert that the structure of FDT is determined by a foam-like topology of the vorticity field lines where the prime role is played by the hierarchy of helical fluctuations. The active production of turbulence in this picture proceeds outside of these fluctuations and concentrates in space of fractal dimensionality. Presently, we have a rather extensive experimental data to support our view. Further experiments are underway.

(ii) Interfacial Mechanics.

(a) A mechanism for the development of the deformation patterns commonly observed on the surfaces of biological cell plasma membranes was suggested. In this mechanism, the membrane is treated as a viscoelastic continuum and a chemical reaction network on the surface of the membrane regulates the membrane elasticity.

(b) Hydrodynamic waves induced by chemical reactivity waves was studied. Results indicate that a wave of chemical reactivity derived from a multistable chemical reaction on the surface of a thin liquid film is able to induce a hydrodynamic wave in the film through the Marangoni tractions due to the reactivity wave.

(c) The classical linear capillary instability of a thin fluid filament surrounded by a bulk fluid was investigated for the case in which the filament is in steady shear flow. Results indicate that a nonlinear interaction between the shear flow and the capillary forces can, under certain conditions, stabilize the developing linear instability.

STATE UNIVERSITY OF NEW YORK
Department of Mechanical and Aerospace Engineering
Buffalo, New York 14260

46.	THE EFFECT OF AIR FLOW INSIDE A PNEUMATIC TIRE ON TEMPERATURE BUILDUP AND ROLLING RESISTANCE William J. Rae	$86,000	01-01 84-1

The objective of this study is to quantify the effects of air flow and heat transfer inside a pneumatic tire on the temperature buildup and rolling resistance of the tire. The approach being followed has three phases: in the first, detailed measurements are being made of the flow velocities inside a tire under typical operating conditions. The principal experimental apparatus being used in these experiments is a set of hot-wire anemometers. In addition, pressures and temperatures will be measured at selected points. In the second phase, a computer program for predicting this flow will be developed, and its results compared with the experimental data. During the third phase, an energy-balance model will be developed, by means of which the flow and heat-transfer information developed in the first two phases will be translated into quantitative knowledge about energy losses due to the air flow. The overall result expected from this work is a method for assessing quantitatively the energy balance of the tire, as affected by load, road speed, inflation pressure, and other parameters.

546

NORTHWESTERN UNIVERSITY
Chemical Engineering Department
Evanston, Illinois 60201

47. CONVECTIVE BOILING HEAT TRANSFER $ 0 01-02
IN NARROW ANNULAR GAPS 81-3
S. G. Bankoff, R. S. Tankin,
M. C. Yuen

Commercial nuclear steam generators are subject to accelerated stress-corrosion due to thermal cycling in the crevices between the boiler tubes and tubesheets, probably resulting from periodic rewetting and dryout. The objective of this research is to study boiling heat transfer in these short narrow gaps, using a two-loop system, with the primary water side operating up to 17 bars, and the secondary steam-water side up to 7 bars. Heat transfer coefficients over a range of inlet qualities and flow rates have been measured. Improved correlations, taking into account the crevice L/D effect, have been obtained. It is found that bubble flattening and coalescence occur throughout the nucleate boiling range. Hence the onset of transition boiling, which marks the heat flux, is far more gradual than in conventional forced-convection boiling. The dependence on gap thickness and on Reynolds number is also much greater than in wide gaps.

NORTHWESTERN UNIVERSITY
Department of Civil Engineering
Evanston, Illinois 60201

48. EFFECTS OF CRACK GEOMETRY AND NEAR-CRACK MATERIAL BEHAVIOR ON SCATTERING OF ULTRASONIC WAVES FOR QNDE APPLICATIONS — $55,000 — 01-03, 83-3
J. D. Achenbach

Among the methods of quantitative non-destructive evaluation of structural elements, the method based on scattering of ultrasonic (elastic) waves by flaws is particularly useful. The work on this project is concerned with applications of the scattered field approach to the detection of a cracklike flaw, and to the determination of its location, size, shape, and orientation. Interior, as well as surface-breaking and near-surface cracks are considered. The usual mathematical modeling of ultrasonic wave scattering by cracks is adjusted to account for several typical characteristics of fatigue and stress-corrosions cracks, and the environment of such cracks. Effects due to crack-face roughness, crack-closure and crack-face interactions are considered, as well as global anisotropy. Local anisotropy and inhomogeneity due to near-tip voids, and the effect of a zone of plastic deformation near a crack tip will also be investigated. Parametrical studies are expected to display the masking of characteristic "crack-like" features of the scattered field by a spectrum of signals due to deviations from an idealized crack geometry and idealized material behavior. Progress has been made on the effects of crack-face interactions and global anisotropy.

OAK RIDGE NATIONAL LABORATORY
Engineering Physics and Mathematics Division
Oak Ridge, Tennessee 37831

49.	CENTER FOR ENGINEERING SYSTEMS ADVANCED RESEARCH (CESAR) C. R. Weisbin	$400,000	01-03 84-10

The Center for Engineering Systems Advanced Research (CESAR) conducts interdisciplinary long-range research and concept demonstration of intelligent machines that will operate in unstructured hostile environments related to energy production. CESAR provides a framework for merging concepts from the fields of artificial and machine intelligence with advanced control theory. Emphasis is currently directed toward real-time decision making using specialized computer architectures and concurrent processing, model development and solution for coordinated manipulation of flexible arms, and automated sensitivity theory for model simplification and parameter identification. Longer-range goals and priorities will be guided by the final report of the DOE/ORNL sponsored workshop which identified and prioritized research issues in the disciplines of (1) sensors (non-vision), (2) vision, (3) mechanisms, dynamics and controls (4) knowledge representation, reasoning and cognition, and (5) man-machine communication.

During this past year, a prototype mobile robot (designated HERMIES) was designed and built to serve as a focus and concept test-bed for studying how systems might deal with resource constraints (e.g., time), goal conflicts, imprecise information, emergency interrupts, coordinated manipulation and learning. CESAR research in FY'84 was documented with initial publications concerning real-time strategic planning (Robot Operating System, minimal cut-set theory), computer assisted symbolic generation of manipulator equations, concurrent computation of complex equations (such as those for inverse dynamics), robotic control of teleoperator arms, and development and validation of an automated implementation of adjoint perturbation theory for systematic parameter identification, model simplification and uncertainty analysis.

PACIFIC NORTHWEST LABORATORY
Engineering Physics Department
Richland, Washington 99352

50. HOLOGRAPHIC INVESTIGATION OF THERMAL-NONEQUILIBRIUM VAPOR GENERATION IN TWO-PHASE FLOWS $135,000 01-02 81-3
J. M. Bates, B. B. Brenden,
J. L. Daniel

The principal objective of the research is to gain a basic understanding of the thermal nonequilibrium vapor generation process. Nonequilibrium vapor generation is known to have major implications in the analysis of postulated Loss of Coolant Accidents (LOCA) for light water nuclear reactors as well as being important to the analysis and development of alternate energy sources such as geothermal, liquified natural gas, and solar. Single and double pulse holographic optical recording techniques and associated image analysis capabilities are being utilized to permit detailed three-dimensional characterization of two-phase flow fields in regions of thermodynamic nonequilibrium. Two-phase flow fields will be formed in rapidly depressurizing, recirculating flow through a specially designed convergent-divergent nozzle assembly. The first two years of the multi-year project were devoted to optimizing holocamera systems, developing appropriate software for a semiautomated contrast scanner/image analysis system, and designing and procuring hardware for tests in a closed loop high pressure/temperature thermal hydraulic facility. Data acquisition and reduction began in FY 1984 and will continue in FY 1985. The observed periodic nature of the vapor generation phenomena have dictated a redesign of the holocamera system.

UNIVERSITY OF PENNSYLVANIA
Department of Electrical
Engineering and Science
Philadelphia, PA 19104

51. HIGH TEMPERATURE CHEMICALLY SENSITIVE ELECTRONIC DEVICES $100,000 01-03
82-3
J. N. Zemel, I. R. Lauks,
S. Yuen, J. Wei

Monitoring the chemical environment in an aqueous saline solution is a major problem in geothermal environments. Additionally, the kinetic behavior of aqueous solutions in the temperature range from 0-250°C and pressures from 0-5000 psi have not fully investigated. The purpose of this program is to develop the scientific and technological knowledge which will permit real time analysis of the chemical behavior of aqueous saline solutions in this temperature and pressure regime. The approach adopted has been to develop a chemically sensitive electronic device based on a specially designed and constructed gate controlled diode (ICD). These devices have been demonstrated to operate up to 200°C. IrO reactively sputtered films have been shown to survive 200°C at 4000 psi in distilled water for periods in excess of four hours without any observable degradation. In the past six months, a four element (ion) structure has been designed and preliminary data obtained on its operation. Continuing measurements on IrO stored in water for a year showed that the layers would survive with a pH response that was reproducible to better than 10mV. Continued efforts are planned on characterizing the IrO layers and completing the four element sensor.

UNIVERSITY OF PENNSYLVANIA
Department of Mechanical Engineering
and Applied Mechanics
Philadelphia, Pennsylvania 19104

52. CRACK-TIP FIELDS FOR MATERIALS WITH EXPONENTIAL-LAW-CREEP BEHAVIOR AT HIGH STRESS $67,000 01-04 83-2
John L. Bassani

This research is concerned with elastic-viscoplastic analyses of cracks under creep conditions, with particular emphasis on the influence of the assumed stress dependence on the creep strain-rate. The total strain-rate is taken as the sum of linear elastic and hyperbolic-sine-creep rates: $\dot{\varepsilon}=\dot{\sigma}/E + \dot{\varepsilon}_0 \{\sinh(\sigma/\sigma_0)\}^n$. Around the tip of a sharp notch in a material described by this law the creep strain-rates are much greater than the elastic ones. The spatial asymptotic analysis based upon a hodograph transformation demonstrates that the notch-tip stress intensification is weaker and the strain-rate intensification is stronger than for a power-law creeping material. The complete time-dependence of the crack-tip fields under Mode III small-scale-yielding conditions has been investigated numerically. Accurate finite element solutions demonstrate that in small-scale yielding, relaxation around the crack tip follows $\sigma \dot{\varepsilon} \times 1/t$ as in the power-law case. This result can be proven in the case of relatively low applied load levels, that is for small values of the elastic stress intensity factor, K^{III}. The fact that this holds for large values of K^{III}, in which case the stresses are everywhere outside the power-law regime, is very interesting if not surprising. Attempts to prove this limit from similarity analysis have not been successful. This research will conclude with an analysis of crack-tip fields under plane-strain Mode I conditions.

PHYSICAL SCIENCES INC.
Research Park, P. O. Box 3100
Andover, Massachusetts 01810

53. EXPERIMENTAL AND THEORETICAL STUDIES OF CONDENSATION IN MULTICOMPONENT SYSTEMS $60,000 01-06
84-4
M. B. Frish, G. Wilemski

This research program comprises experimental and theoretical studies of nucleation and condensation in multicomponent gas mixtures. The program goals are: 1) to improve basic understanding binary nucleation and droplet growth, 2) to stringently test theories of binary nucleation at high nucleation rates and under nonisothermal conditions, 3) to develop improved theories where needed, 4) to enlarge the data base for systems of both fundamental and practical interest, and 5) to provide reliable means for predicting the behavior of mixtures used in practical applications such as turbomachinery. Experimentally, gas mixtures will be cooled in a supersonic nozzle to obtain much higher binary nucleation rates than have previously been studied. The nozzle is designed to insure that steady state nucleation occurs and to give satisfactory spatial resolution of the temperature profile. Laser light scattering will be the primary means of detecting nuclei as small as 10Å in radius and of monitoring droplet growth. By varying the amount of inert carrier gas used, both isothermal and nonisothermal nucleation will be studied. Design of the flow and optical systems is complete and construction is in progress. A new thermodynamic theory of binary cluster composition has been developed. Calculations with this theory have established the feasibility of using bulk liquid mixture surface tensions to compute nucleation onset (for small rates) in alcohol-water mixtures, thus removing a severe deficiency of classical binary nucleation theory.

ROCKEFELLER UNIVERSITY
Department of Physics and Mathematics
1230 York Avenue
New York, New York 10021

54.	SOME BASIC RESEARCH PROBLEMS RELATED TO ENERGY Kenneth M. Case, E.G.D. Cohen,	$ 0	01-06 81-3

This project is concerned with investigations of three specific areas: 1) The prediction and evaluation of thermophysical data of fluids and fluid mixtures, 2) The statistical problems which arise in oil exploration, and 3) Study of the applications of nonlinear evolution equations. Work is underway to construct a model which can give a first approximation to the transport properties of fluid mixtures in their dependence on size and mass of the constituent particles. Work is also underway to develop and test various methods of estimating the number of oil pools in an area from a number of random drillings. The nonlinear evolution equations being investigated describe a very large number of energy related processes. One such equation, the so-called Sine-Gordon equation, has been under study and a number of previously unknown results for the equation have been found.

SANDIA NATIONAL LABORATORIES
Device Research Division
Albuquerque, New Mexico 87185

55. HIGH TEMPERATURE ELECTRONICS $110,000 01-03
R. J. Chaffin, L. R. Dawson 80-6
D. R. Myers, T. E. Zipperian

The project addresses fundamental engineering questions relevant to the development of high-temperature (up to 500°C) electronics for energy technologies. Included are sensors, passive components, and active semiconductor devices which provide electronic gain. The FY84 work has concentrated on electronic devices fabricated from heterojunctions formed from gallium arsenide (GaAs) and aluminum gallium arsenide ($Al_xGa_{1-x}As$). This material system, although inferior in its high temperature properties to materials previously reported like gallium phosphide (GaP) or aluminum gallium phosphide ($Al_xGa_{1-x}P$), may prove to be a more manufacturable technology. Within the $GaAs/Al_xGa_{1-x}As$ system, heterojunction diodes have shown excellent rectification to 450°C. This operational temperature is approximately 100°C less than that of GaP/Al_xGa_{1-x}-P heterojunction diodes but still over 150°C higher than that of comparable silicon or bulk GaAs devices. More complicated $GaAs/Al_xGa_{1-x}As$ heterojunction transistors and switching devices are also being investigated. Initial results from this project have shown that it is feasible to build active solid-state semiconductor devices for high-temperature service. Future plans include developing stable metallization systems for these devices and developing device geometries and processing techniques compatible with a high-temperature integrated circuit technology.

SANDIA NATIONAL LABORATORIES
Combustion Sciences Directorate
Thermofluids Division
Livermore, California 94550

56. CONVECTIVE DROPLET VAPORIZATION AND COMBUSTION $160,000 01-05
81-3
B. R. Sanders, H. A. Dwyer,
A. R. Kerstein

The technical goal of this project is to develop a complete analysis of liquid droplet vaporization and combustion processes through single droplet modeling and a statistical approach to multidroplet interactions. First, an analysis of liquid droplet vaporization and combustion will be developed by solving the coupled shear-driven recirculation flow within the droplet and the external convective gas-phase flow past the droplet, where a differential velocity exists between the droplet and free stream. Second, a statistical approach will be developed to study the combustion of a large ensemble of droplets whose locations and sizes are randomly distributed. The detailed solution of individual droplet heating and vaporization will be used as empirical inputs to the statistical spray combustion model. The single droplet numerical model has been extended to include variable transport properties in liquid and gas phases, complete separated fluid mechanics, and mass transport at the droplet surface. Additionally, a combusting spray was modeled where droplet interactions influence the connectedness of the flame zone (localized pockets of flame vs. a single connected continuum). Percolation theory has been used to identify the transition between these regimes, and to derive the dynamics of this transition as burnout proceeds in a simple spray geometry. This is the first known application of statistical methods to the problem of flame zone connectedness, a previously unresolved question of long standing.

SCIENCE APPLICATIONS, INC.
1200 Prospect Street, P. O. Box 2351
LaJolla, California 91038

57. ASPECTS OF TURBULENCE IN NONLINEAR SYSTEMS $72,000 01-06
E. Frieman 84-3

The basic goal of this program is to advance the understanding of flow and transport in turbulent systems. A central strategy is to exploit the distinct sets of temporal and spatial scales exhibited by most physical systems. The plasma system is chosen as a specific example in which to develop and demonstrate these methods.

The program has been broken down into five tasks: (1) The first task is to understand the relation between the various gyroradius kinetic theories. (2) The second task is to derive these gyrokinetic equations from the viewpoint of contemporary Hamiltonian dynamics. The relation between divergencies in the generating functions (for Lie transform theory) and resonances in the solutions to the nonlinear perturbative equations of motion will also be explored in this task. (3) The third task involves application of modern procedures to the resulting nonlinear systems arrived at in the first two tasks. Field theoretic techniques will lead to expansions which might be parameterized in terms of the linearization amplitude and the ratio of Larmor theory. (4) The fourth task involves the investigation of applying renormalization group theories to these equations to yield nonperturbative relations among correlation functions. The nature and distinction between intrinsic and extrinsic stochasticity will also be examined. (5) Lastly, application of the concepts and lessons learned to a broader class of turbulent systems will be considered.

SCIENTIFIC SYSTEMS, INC.

34 Rindge Avenue Extension
Cambridge, Massachusetts 02140

58. CHAOTIC DYNAMICS IN FEEDBACK SYSTEMS $65,000 01-03
J. Baillieul, R. W. Brockett 82-3
N. Kopell

The objective of this research effort is to study chaotic motions occuring in certain classes of dynamical systems which arise in the study of feedback control systems, electric power conversion circuitry and various other engineering applications. Part of the effort is focused on a simple class of differential equations whose coefficients depend piecewise linearly on the state. Because this is a simpler class of dynamical systems than others (such as the well known Lorenz system) which have been widely studied recently, it is possible to obtain especially accurate simulations of system trajectories. On the other hand, numerical simulations that have been carried out indicate very interesting qualitative features of the dynamics of such systems, and there is evidence of a strange attractor in a very simple third order system. Specific research is aimed at these and other classes of models in three areas: (i) the use of singular perturbations techniques to analyze first return maps, (ii) the use of difference equations to study to qualitative behavior of "chaotic" differential equations, and (iii) the use of input/output analysis (particularly various control theoretic techniques involving Nyquist plots, describing functions, etc.) to study the qualitative behavior of feedback models.

SKF INDUSTRIES, INC.
1100 First Avenue
King of Prussia, PA 19406-1352

59. MECHANICAL INTERACTIONS OF ROUGH SURFACES $100,000 01-06
J. I. McCool 84-3

This program is aimed at developing fundamental information and resolving a number of issues that impact the design of mechanical systems in which surface microtopography per se or events which occur on the microgeometric scale play a critical role.

The work is organized into two distinct tasks:

In Task I, a rig designed and built by SKF is being used to provide optical interferograms of the lubricated contact of rough surfaces along with measurements of the traction transmitted under conditions of combined rolling, sliding and spinning. These tests will serve to explore the limitations of predictive models of film thickness, traction, and the frequency of asperity contact interactions and micropitting in the so called partial EHD regime wherein the thickness of the lubricant film separating the bodies is of the same order as the surface roughness amplitudes.

The objective of Task II is to develop guidelines and techniques for the digital processing of surface roughness data generated in analog form by a stylus profile instrument.

Issues to be addressed are: filter bandpass selection, record length and sample spacing, spatial vs. frequency domain estimation, type of digital filtering and the effects of preprocessing.

UNIVERSITY OF SOUTHERN CALIFORNIA
Department of Physics
University Park
Los Angeles, California 90089

60.	A STUDY OF GAS-SURFACE ENERGY EXCHANGE PROCESSES J. A. Kunc, D. E. Shemansky	$70,000	01-06 83-3

The objective of this theoretical research program is to study the fundamental characteristics of gas-surface energy exchange reactions. The interaction process refers to low density conditions in the gas component and therefore has general application to a number of disparate disciplines, including the maintenance of clean high vacuum systems for research in subjects such as fusion reactions, and many other important areas in engineering and technology. The approach to the calculations is to construct accurate theoretical models of the solid structure on a microscopic scale, and account for the many body gas surface physical interaction using Monte Carlo techniques. Calculations are presently underway involving 60-dimensional He - Alpha quartz, and H - Alpha quartz interaction systems in which entrappment, adsorption and scattering events are accumulated to describe the aggregate interaction probabilities. One of the fundamental questions to be examined is the relationship between the physical scale interaction potential of the individual gas atom - solid atom pair and the effective mean potential of the gas - surface interaction many body system. Attempts to establish this relationship in earlier work have tended to be empirical in nature because of the difficulty of dealing with a many body system. A modification of the present energy exchange computer codes has allowed calculation of the gas surface potential curve in an exact manner limited by statistical fluctuations in the Monte Carlo regime. Potential curves have been calculated for both He and H interactions for particular pairwise interaction parameters. The results are in process of publication, while work continues on the effect of the physical parameters on the shape of the curve.

STANFORD UNIVERSITY
Department of Chemistry
Stanford, California 94305

61. EFFICIENCY OF CHEMICAL AND THERMAL ENGINES $97,000 01-06
J. Ross 82-4

Research is concerned with the issue of the enhancement of power output in thermal and chemical engines by means of external perturbations of constraints coupled to nonlinearities of the mechanism of the engine. The possibility has been shown of the increase in power output of the thermal engine driven by a chemical reaction by means of external periodic variation of pressure, temperature and mass flux for the same average chemical throughput as the unperturbed (steady or periodic) state. Since the power output of an engine is necessarily accompanied by dissipation due to irreversible processes essential for power production, an increase in the power output by means of external perturbations is accompanied by a decrease in the rate of entropy production. There exists particular frequencies of external perturbations at which resonance effects lead to enhancement of power output. A linear analysis is possible by analytic methods but the full nonlinearities need to be treated by numerical methods. Research is planned on optimization of cycles for combined thermal and chemical engines, and the search for upper limits of the efficiency of chemical engines with non-zero throughput (reaction rates) of monotonic and oscillatory reactions.

STANFORD UNIVERSITY
Department of Civil Engineering
Stanford, California 94305

62. MOMENTUM AND HEAT TRANSFERS IN A COMPLEX, BUT WELL-DEFINED TURBULENT FLOW $67,000 01-03
84-3
R. L. Street

A basic study of a three-dimensional, variable density, recirculating flow is being conducted in a lid-driven cavity. A unique facility has been created to provide an extremely well-regulated flow. Water is the working fluid. The objectives of the research are to provide 1) a complete data base for a range of conditions (laminar, turbulent, forced convection, etc.) in a complex recirculating flow, 2) deeper insight into the physical processes governing heat and momentum transport in such flow, and 3) a critical evaluation of the performance of numerical simulation models in predicting the experimental results. Flow and temperature visualization has been carried out for 1) homogeneous, 2) stably stratified and 3) naturally buoyant flow conditions. General flow features have been established for Reynolds numbers up to 10,000, e.g., the number of identifiable eddy structures, the presence of Taylor-Görtler vortices, and the strength and the development of the thermocline in the stratified cases. LDA velocity measurements have been obtained and compared with both two- and three-dimensional numerical codes. Several codes simulate the experimental results for laminar flows quite well except for the Taylor-Görtler vortices, which have been reproduced successfully so far by only two three-dimensional codes with fine grids. Turbulent flow cases and code modifications are to be examined. Temperature and heat flux measurements are being made. Temperature and velocity correlation data will be obtained for turbulent flow cases using LDA and the temperature rig simulaneously.

STANFORD UNIVERSITY
Edward Ginzton Laboratory
Stanford, California 94305

63. HIGH FREQUENCY TRANSDUCERS G. S. Kino	$20,000	01-03 81-3

This year, a new theory has been developed for cross-coupling in acoustic transducer arrays, used for acoustic imaging. Cross-coupling changes the pulse response and the angular response of the arrays. The results compare very well with theory. This is an entirely new theoretical technique applicable to acoustics devices for NDT, medical and sonar arrays, as well as to electromagnetic and antenna arrays. Techniques for reducing cross-coupling have also been suggested and tried with some success.

New developments have been made of air transducers operating at 1 and 2 MHz in air. These are used for precision measurements of distance in air. This is of great importance for diamond turning, robotic applications, nondestructive testing and profile measurements in precision manufacturing.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Stanford, CA 94305

64.	HEAT TRANSFER EFFECTS OF LONGITUDINAL VORTICES EMBEDDED IN A TURBULENT BOUNDARY LAYER John Eaton	$49,000	01-02 83-3

Large-scale longitudinal vortices can be developed in a turbulent boundary layer by a variety of mechanisms. Such vortices can cause significant local augmentation of the heat-transfer rate. The objectives of the present study are (i) to examine the effects of an isolated vortex independent of other interfering phenomena and (ii) to determine what physical mechanisms are responsible for the heat-transfer augmentation. Experiments are being conducted in a two-dimensional, boundary-layer wind tunnel. The vortex is formed by a half delta wing attached normal to the test wall and at an angle of attack to the oncoming flow. The spatially resolved heat-transfer coefficient is measured using a constant-heat-flux foil surface with 160 thermocouples for surface-temperature measurements. All three components of the mean velocity are measured using a four-hole pressure probe, and turbulent stresses are measured using hot wires. A typical vortex decays very slowly in a zero pressure gradient flow and causes a peak heat-transfer augmentation of around 25%. Mean-velocity data suggest that the augmentation is associated with local thinning of the boundary layer by the vortex. In the next phase, skin-friction and near-wall velocity data will be obtained to document the effect of the vortex on the sublayer.

STANFORD UNIVERSITY
Mechanical Engineering Department
Stanford, California 94305

65. A NEW METHOD FOR PREDICTING MULTIAXIAL FATIGUE $0 01-04

D.V. Nelson 81-3

The objective of this project is to develop an improved method for predicting the fatigue life of components which experience multiaxial cyclic stresses. Using available data in the literature, an evaluation of existing methods used in design analysis (e.g., the procedures of the ASME Boiler and Pressure Vessel Code) showed that such methods are often non-conservative when loadings are applied out-of-phase, which is frequently the case in service. The evaluation also showed that two new approaches are more accurate than existing ones as well as being conservative. The first approach predicts life based on maximum shear strain amplitude modified by a fraction of the normal strain amplitude acting on the plane(s) which experience maximum shear. The second relates multiaxial cyclic plastic work to life, using only uniaxial fatigue and cyclic stress-strain properties as input to the computations. Of the two new approaches, the plastic work method appears somewhat superior, and a test program is being completed to provide a critical check of it. Specimens of A533B pressure vessel steel have been tested in deflection-controlled, combined bending and torsion, applied both in-phase and 90 degrees out-of-phase, at two different fixed ratios of bending-to-torsion strain, and at a number of different strain amplitudes to produce lives ranging between 10^2 to 10^6 cycles. The life to formation and subsequent growth of cracks from 0.1 mm size till fracture (10 mm size) have been recorded. Based on test results to date, it appears that the relative fatigue damage of in-phase vs. out-of-phase loading, as well as crack growth behavior, depends on both the bending-to-torsion ratio and the strain amplitudes being applied. For all test combinations studied, the life to formation of 0.1 mm sized cracks has been correlated well by the plastic work method, but not by conventional approaches. The growth of cracks to mm size has also been correlated reasonably well by an approach based on the use of the ΔJ^{I} and ΔJ^{III} elastic-plastic fracture mechanics parameters.

STANFORD UNIVERSITY
Department of Mechanical Engineering
Division of Applied Mechanics
Stanford, California 94305

66. ENERGY CHANGES IN TRANSFORMING SOLIDS $70,000 01-04

George Herrmann, David M. Barnett 82-4
A. Golebiewska-Herrmann

Energy changes in deformable solids accompany and control a variety of processes related to void formation, void growth, damage and fracture. A powerful method for characterizing such changes is based on material conservation and balance laws. The basic quantity of interest in this connection is the so-called material momentum tensor, which plays a role analogous to the stress tensor. Several problems have been recently completed and are currently under study. They include calculation of energy changes associated with boundaries and interfaces, introducing the concept of material traction, analogous to (classical) physical (or spatial) Cauchy traction, and investigating a variety of geometries. Another problem concerns the properties of the material momentum itself. In linear elasticity, this quantity is asymmetric. It is established, however, that in a fully nonlinear theory, this tensor is symmetric and proper linearization leads to a new symmetric material momentum even in classical linear elasticity, whose properties have yet to be fully explored.

The calculation of the redistribution of impurity atoms about a uniformly gliding edge dislocation is currently being performed. The local impurity concentration is governed by a non-linear diffusion equation which must be solved by finite difference techniques; the source of non-linearity is essentially due to the fact that only one impurity atom is allowed to occupy any given substitutional site. Once the concentration variation is obtained, the solute drag force on the dislocation can be determined from Lothe's power dissipation theorem. We then intend to study solute redistribution near a uniformly climbing edge dislocation and near dislocations in non-uniform motion.

We have succeeded in developing a proper prescription for defining chemical potential at the interface between two dissimilar stressed elastic solids; this prescription accounts for differences in specific volumes of the two media and is valid for quite general stress states. We have begun to examine the relationship between our expression for chemical potential and the "force on an interface" as first deduced by Eshelby.

STEVENS INSTITUTE OF TECHNOLOGY
Department of Physics and Engineering Physics
Hoboken, New Jersey 07030

67. INVESTIGATIONS OF TRANSITIONS FROM ORDER $40,000 01-06
TO CHAOS IN DYNAMICAL SYSTEMS 83-3
George Schmidt

The transition from order to chaos in dynamical systems of few degrees of freedom are studied, using theory, numerical computations and a simple laboratory experiment as tools of this investigation. In particular different routes to chaos in Hamiltonian systems are investigated. Increasing evidence has accumulated that the universal bifurcation sequence is just one of many possible scenarios. A systematic way is developed to deal with a variety of Hamiltonian systems, that show chaotic behavior. The next step is the investigation of dissipative systems of few degrees of freedom. How is the behavior of a Hamiltonian system modified when damping is introduced rendering the system non Hamiltonian? What is the fate of stable periodic orbits as dissipation is increased, and how do strange attractors arise? Driven, damped nonlinear oscillators are examples of systems of that type. It is hoped that a thorough understanding of simple systems exhibiting great complexity, will shed light to a better understanding of more complex systems which are as yet inaccessible to detailed study.

UNIVERSITY OF TEXAS AT AUSTIN
Department of Physics
Austin, Texas 78712

68. PERTURBATION AND CHARACTERIZATION OF NONLINEAR PROCESSES Harry L. Swinney and J. Swift	$80,000	01-06 83-4

In this study techniques are being developed to characterize regular and chaotic behavior in nonlinear systems. Although recent theoretical and experimental studies have shown that nonlinear nonequilibrium processes often exhibit nonperiodic behavior, it is difficult to relate these results to nonlinear systems in industry and in nature because research thus far has concerned primarily deterministic systems with no perturbations, while noise is always present for real systems. Moreover, the observed nonperiodic behavior has not been quantified, so experiments cannot be easily compared with one another and with theory. In this research we are addressing these problems by (1) conducting experiments on the Belousov-Zhabotinskii reaction in a well-stirred flow reactor with imposed computer-controlled perturbations, and (2) developing a method to determine from experimental data the Lyapunov exponents that characterize a nonperiodic process. Methods will also be developed for determining from laboratory data other quantities including the fractal dimension and the metric entropy.

UNIVERSITY OF TEXAS AT AUSTIN
Center for Studies in Statistical Mechanics
Austin, Texas 78712

69. BIFURCATIONS AND FLUCTUATIONS IN FAR FROM EQUILIBRIUM SYSTEMS Ilya Prigogine	$18,000	01-06 81-3

In many instances, physico-chemical systems give rise to self-organization and complex behavior. Bifurcations and fluctuations constitute the basic mechanism of evolution far from thermodynamic equilibrium. The purpose of this research is to explore the implications of bifurcations and fluctuations in the modelling, design and stability of complex systems of interest in physics and engineering. Special emphasis is being placed on the following two aspects. First, the effects of temperature fluctuations on the performance of chemical reactors is being examined in connection with the onset of explosive behavior. Second, the coupling between a complex systems and its environment is being considered; the sensitivity of nonlinear systems to small forces embedded in noise is being studied. Previous work has shown the Possibility of a new type of transition induced by environmental noise and external fields. The repercussion of these transitions is being studied for systems involving multiphotonic steps.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY
Depts. of Engineering Mechanics and Mechanical Engineering
Blacksburg, Virginia 24061

70. HEAT TRANSFER IN OSCILLATORY FLOW $100,000 01-02
D. P. Telionis, T. E. Diller 82-4

The response of the velocity field and heat transfer of a single cylinder and bundles of cylinders to forced oscillations of the mean stream is investigated. Parallel experiments are conducted in a wind tunnel and a water tunnel. In the first facility the emphasis is given to heat transfer, whereas in the second the flow is examined in detail via Laser-Doppler Velocimetry and Flow Visualization. Analytical efforts are based on numerical integrations of boundary layer equations and special mathematical tools for modeling the flow and heat transfer in the wake of the cylinders. Special attention is directed at determining the range of parameters in which the overall heat transfer is improved with simultaneous decrease of the flow resistance. Two unsteady wind tunnels have been constructed and a water tunnel was modified for unsteady flow especially for this project. Extensive tests were conducted by measuring the time-averaged heat transfer and the fluctuating velocity fields. For a low-turbulence pulsating flow the changes in the local heat transfer coefficient relative to steady flow are small except near the separation point, even for large pulsation amplitudes. This is in contradiction with most earlier reports, particularly in the wake region. Work is continuing to measure the effect of flow pulsation on heat transfer as a function of freestream turbulence and in the presence of tube bundles. Preliminary pressure and load measurements proved successful. Moreover, a sensor was constructed and calibrated to measure time-resolved, local heat transfer. A finite-element-Navier-Stokes solver was developed to solve the problem of single and multiple cylinders. The models for experiments on bundles of cylinders are being prepared. Experimental and analytical work will proceed in this direction in the next year.

UNIVERSITY OF WISCONSIN
Department of Chemical Engineering
Madison, Wisconsin 53706

71. THE DEVELOPMENT OF PROCESS $90,000 01-03
DESIGN AND CONTROL STRATEGIES 80-6
FOR ENHANCED ENERGY EFFICIENCY
IN THE PROCESS INDUSTRIES
M. Morari, W. H. Ray, D. F. Rudd

The process industries are a major consumer of energy and the improvement of energy efficiency is an important goal. Process modifications aiming at a reduction of energy consumption tend to make a plant more integrated and thus more difficult to operate. In practice, the primary objective is not only steady state energy efficiency but that the plant is flexible, operable and controllable, i.e. resilient. The research goals are to develop design strategies for resilient processes and operating policies for highly integrated plants. The particular subtasks are: 1) Synthesis of resilient energy management networks, 2) Development of control strategies for integrated distillation columns, and 3) Development of control and optimization procedures for systems with high parametric sensitivity (chemical reactors). The latter two tasks involve an extensive experimental verification phase. The development of interactive user-friendly CAD packages incorporating the fundamental theoretical developments are under way.

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Number

01-01

Includes projects concerned with research related to friction and wear. See project numbers:

18, 36, 40, 44, 46.

01-02

Includes projects concerned with research on the effects of turbulence, vibrations and noise, and heat transfer. See project numbers:

2, 9, 11, 13, 14, 19, 20, 39, 41, 47, 50, 64, 70

01-03

Includes projects concerned with research on adaptive control systems, non-linear systems, modeling, sensors for hostile environments, and NDE instrumentation. See project numbers:

1, 3, 8, 16, 22, 24, 25, 27, 28, 31, 32, 34, 37, 38, 43, 48, 49, 51, 55, 58, 62, 63, 71.

01-04

Includes projects concerned with research on the macroscopic aspects of elastoplastic deformations and of crack propagation in structural materials. See project numbers:

4, 23, 26, 52, 65, 66.

01-05

Includes projects concerned with research on dat bases, lean mixture ignitions, and modeling of real combustion systems. See project numbers:

5, 6, 7, 15, 17, 29, 35, 42, 56.

01-06

Includes projects concerned with research on analysis of non-imaging optics, and noise and fluctuations in non-linear systems. See project numbers:

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FOREWORD

The Department of Energy supports research in the geosciences in order to provide a sound foundation of fundamental knowledge in those areas that are germane to the Department of Energy's many missions. The Division of Engineering, Mathematical and Geosciences — part of the Office of Basic Energy Sciences which is under the Director of Energy Research — supports the Geosciences Research Program. The participants in this program include Department of Energy laboratories, industry, universities, and other governmental agencies. Their support, formalized by a contract between the Department of Energy and the organization performing the work, provides funds for salaries, equipment and other materials, and an overhead allowance.

The summaries in this document, prepared by the investigators, describe the scope of the individual programs and detail the research performed during 1983-1984. The Geosciences Research Program includes research in geology, petrology, geophysics, geochemistry, hydrology, solar-terrestrial relationships, aeronomy, seismology, and natural resource analysis, including their various subdivisions and interdisciplinary areas. All such research is related either directly or indirectly to the Department of Energy's technological needs.

INTRODUCTION TO THE GEOSCIENCES RESEARCH PROGRAM OF THE OFFICE OF BASIC ENERGY SCIENCES

The Geosciences Research Program is directed by the Department of Energy's Office of Energy Research, within the Office of Basic Energy Sciences, Division of Engineering, Mathematical, and Geosciences. Research supported by this program may be directed toward a specific energy technology, national security, conservation of the environment, or the safety objectives of the Department of Energy. The purpose of this program is to develop geoscience or geoscience-related information relevant to one or more of these Department of Energy objectives or to develop the broad, basic understanding of geoscientific materials and processes necessary for attaining long-term Department of Energy goals. In general, individual research efforts supported by this program may involve elements of all four objectives.

The Geosciences Research Program is divided into five broad categories:

- Geology, geophysics, and earth dynamics
- Geochemistry
- Energy resource recognition, evaluation and development
- Hydrologic and marine sciences
- Solar-terrestrial-atmospheric interactions.

The following content outline of these categories is intended to be illustrative rather than exhaustive, and will evolve with time. Individual research efforts at the Department of Energy, university, college, corporate, not-for-profit, and other Federal agency laboratories supported by this program frequently have components in more than one of the categories or subcategories listed.

1. Geology, Geophysics, and Earth Dynamics

    A. Large-Scale Earth Movements. Research related to the physical aspects of large-scale plate motion, mountain building, and regional scale uplift or subsidence.

    B. Evolution of Geologic Structures. Research bearing on the history and development of geologic structures (e.g., folds, faults, landslides, and volcanoes) on a local or subregional scale.

    C. Properties of Earth Materials. Research on physical properties of rocks and minerals determined in the laboratory or in the field (in situ) by direct or indirect techniques.

    D. Rock Flow, Fracture, or Failure. Research related to response of minerals, rocks, and rock units to natural or artificially induced stress, including the strain rates that range from those appropriate to drilling to viscoelastic response.

2. Geochemistry

   A. Thermochemical Properties of Geologic Materials. Research related to thermodynamic and transport properties of natural geologic materials and their synthetic analogues. Emphasis is on generic rather than site-specific studies.

   B. Static Rock-Water Interactions. Laboratory-based research on chemical, mineralogical, and textural consequences of interaction of natural aqueous fluids, or their synthetic analogues, with rocks and minerals.

   C. Organic Geochemistry. Research on naturally occurring carbonaceous and biologically derived substances of geologic importance, including research on the origin and development of coal, petroleum and gas.

   D. Geochemical Migration. Research on chemical migration in materials of the earth's crust, emphasizing a generic rather than specific understanding, which may (ultimately) lead to predictive capability. These experimental and theoretical studies focus on chemical transport induced by pressure, temperature, and composition gradients within, between, and by a phase or phases. This component is part of a multiagency (Department of Energy, National Science Foundation, U.S. Geological Survey) joint program.

3. Energy Resource Recognition, Evaluation, and Utilization

   A. Resource Definition and Utilization. The principal goal of this research is to develop new and advanced techniques that are physically, chemically, and mathematically based, for energy and energy-related resource exploration, definition, and use.

   B. Reservoir Dynamics and Modeling. Research related to dynamic modeling of geothermal and hydrocarbon reservoirs in their natural and perturbed (by production, injection, or reinjection) states.

   C. Magma Energy Resources. Field, laboratory, experimental, and theoretical research bearing on the origin, migration, emplacement, and crystallization of natural silicate liquids or their synthetic analogues. These studies emphasize the extraction of energy from such liquids.

   D. Information Compilation, Evaluation, and Dissemination. These research activities are principally oriented toward evaluating existing geoscientific data to identify significant gaps, including the necessary compilation and dissemination activities.

   E. Continental Scientific Drilling Program (CSDP). Research on advanced technology and services as well as scientifically motivated projects concerned with utilizing shallow (0.3 km), intermediate (0.3 to 1 km), and deep (> 1 km) drill holes in the

United States continental crust to (a) obtain samples for detailed physical, chemical, mineralogical, petrologic, and hydrologic characterization and interpretation; (b) correlate geophysical data with laboratory-determined properties; and (c) use the drill hole as an experimental facility for studying crustal materials and processes. The Department of Energy focuses on drilling through an active hydrothermal system (or systems) into a magma chamber or into high-temperature igneous rocks. Research includes aspects of drilling technology development for such hostile environments. Part of a multiagency (U.S. Geological Survey, National Science Foundation, and Department of Energy) coordinated program under the aegis of an Interagency Accord on Continental Scientific Drilling.

4. Hydrologic and Marine Sciences

   A. Ground Water Hydrology. Research related to chemical and physical principles underlying the flow of water through porous and permeable rocks near the earth's surface.

   B. Fresh Water Systems. Research on the chemistry, physics, and dynamics of fresh water systems, including streams, rivers, and lakes.

   C. Oceanography. Research involving materials and processes of the marine environment. Principal emphasis is on geological, geophysical, and geochemical research related to rocks and sediments beneath the water column.

5. Solar-Terrestrial-Atmospheric Interactions

   A. Magnetospheric Physics. Research directed toward developing a fundamental understanding of the interactions of the solar wind with the terrestrial magnetic field. Research related to the earth's magnetosphere as a model magnetohydrodynamic generator and associated plasma physics research.

   B. Upper Atmosphere Chemistry and Physics. Research on thermal, compositional, and electrical phenomena in the upper atmosphere, and the effects induced by solar radiation.

   C. Solar Radiation. Research on the solar constant, spectral distribution, and characteristics of solar radiation of the earth, including the long-term effects of solar radiation on the climate.

   D. Meteorology and Climatology. Interrelationships of weather and climate with energy systems.

PART I

ON-SITE

Contractor: ARGONNE NATIONAL LABORATORY
Argonne, Illinois 60439

Contract: 109 ENG 38

Title: Geosciences Program

Person in Charge: F. A. Cafasso and M. J. Steindler

Scope of Work

The Geosciences program at Argonne National Laboratory is focused on research in the areas of geochemical migration and mineral thermochemistry. In the migration area strong emphasis is placed on developing an understanding of the chemistry underlying actinide element transport in geomedia. Studies of the thermodynamics, kinetics and mechanisms of actinide complex formation reactions with organic compounds (e.g., humic and fulvic acids) and inorganic constituents in ground (e.g., $CO_3^=$, $SO_4^=$) are being pursued in this connection. Analytical studies of hydrothermally-altered materials are also in progress in an attempt to describe the more general phenomenon of trace element migration in rock-water systems. As research in this program area advances, investigations of rock surface reaction chemistry are expected to become prominent. The thermochemistry part of the program is largely focused on measuring, by a variety of calorimetric methods, the thermodynamic properties of zeolites and related materials. The intent is to develop thermodynamic-structure correlations for these materials and to use the data to explain mineral equilibria.

A. Trace Element Migration in the Earth's Crust (M. Seitz, N. Sturchio, S. Boggs, Jr., and D. Livermore)

An understanding of the distribution and mobilization of trace elements in natural rock-water systems is fundamentally important and is part of the basis for developing rational policies regarding the management of our environment and the evaluation and exploitation of our energy and minerals resources. In this program, we are currently concentrating on two main areas of research: (1) chemical mobility during hydrothermal alteration in active geothermal systems, and (2) the effects of organic compounds in groundwaters on the mobility of heavy elements.

Active geothermal systems provide excellent opportunities for the study of chemical mobility in rock-water systems at relatively high temperatures. This is especially true when rock cores and thermal water (or brine) samples are available from various depths and physical conditions are known. We are now performing a detailed study of hydrothermally altered rhyolitic vitrophyre samples from the Y7 and Y8 shallow research drill holes in

Yellowstone National Park, using electron microprobe, instrumental neutron activation analysis, inductively-coupled plasma atomic emission spectrometry, and mass spectrometry. This work is being done to quantify the chemical mobility concomitant with hydrothermal alteration in these rocks at temperatures of 110°-160° C. We have also analyzed several thermal water samples from the vitrophyre unit in these holes. In a separate study, granite from the 2 km deep drill hole at the Marysville Geothermal Anomaly, Montana, is being investigated to determine the effects of protracted interaction between this rock and the coexisting 95°C dilute sodium bicarbonate-sulfate water.

Organic compounds in groundwaters are known to form stable complexes with heavy elements. We are now investigating the effects of dissolved organics on the distribution ratios of 237-neptunium and 241-americium between basalt and groundwater, using both natural and synthetic groundwater compositions at 25° and 90°C. Special techniques for studying these effects in natural groundwaters are being developed. This work will have important implications regarding the influence of groundwater composition in the transport properties of hazardous waste elements in groundwater aquifers. In related work, we have examined the mobility of phenols in dolomite aquifers. Also under investigation is the use of catalysts in low temperature geochemical experimentation.

B. Migration of Heavy Element Chemical Species in Geologic Media

(F. Schreiner and A. M. Friedman)

The mechanisms of transport of heavy elements in natural geologic formations determine the rate and extent of their dispersal, and the potential localized concentration of these elements in the environment. The objective of the present program is the investigation of the chemical factors that are important in the transport of elements with atomic numbers of 92 and beyond. Chemical properties of importance include redox and hydrolysis equilibria and complex formation. To unravel the complex aggregate of physicochemical interaction modes a number of techniques are being utilized. Oxidation states and reaction rates are determined spectrophotometrically, and equilibrium parameters are established by calorimetry. Rate measurements are made on the microsecond time scale by using the temperature jump technique. The acquired data should provide information potentially useful in the assessment of the safety of nuclear waste repositories, and in the modeling of dispersion patterns for hazardous radionuclides after accidental release.

In recent months calorimetry of the system of complex uranium carbonates has received special attention, along with enthalpy measurements on the reaction of uranyl (VI) ions with such common anions as chloride and sulfate. The calorimeter used for these measurements is a commercial titration microcalorimeter modified for special use with radioactive elements. The instrument is capable of measuring heat releases to ± 0.0005 K-degrees. The results show the calorimetric enthalpies for the carbonato complexes of uranium to be consistent with published equilibrium data based on potentiometric and spectrophotometric measurements. Literature values for the equilibrium constants of the stepwise formation of the dicarbonato- and the tricarbonato uranate ions are 10^{14} and 10^{18}, respectively, indicating very high stabilities for the complex ions. The bond energy for attachment of a carbonato group to the uranyl ion deduced from our calorimetric measurements is near 29 kilojoules, confirming the strong affinity of the carbonate group to the uranium central atom. Calorimeric measurements in the future will concentrate on the complexing reactions of neptunium and plutonium in systems analogous to the uranium systems. At the same time spectrophotometric techniques will be used to identify the reacting species and to establish kinetic parameters. By comparative evaluation of the chemistry of the closely related elements uranium, neptunium, and plutonium we expect to develop correlations which can be used to predict the unknown behavior of transuranium elements in geologic formations.

C. Thermochemistry of Geothermal Materials (P. A. G. O'Hare and G. K. Johnson)

The objective of this program is to measure precisely, by calorimetry, thermodynamic properties of zeolites, silicates, and structurally related compounds. Materials selected for study are often key components of geologic ensembles, they may have real or potential technological value, or they may be of basic scientific interest in terms of structure or chemical bonding. Calorimetric techniques are as follows: solution calorimetry in aqueous HF for the determination of enthalpies of formation, $\Delta_f H_m^o$; low-temperature Calorimetry (5-350 K) for the determination of heat capacities, $C_{p,m}^o$; and the derived standard entropy, S_m^o; drop calorimetry ($T \geq 350$ K) for the determination of enthalpy increments, $H_m^o(T) - H_m^o(298.15)$, and the derived $C_{p,m}^o$; and differential scanning calorimetry for the determination of $C_{p,m}^o$ and temperatures and enthalpies of transition. Measurements cover the temperature range from 5 to 1500 K or the upper temperatures limit of stability.

Based on our published value for the Gibbs free energy of formation of analcime we have been able to estimate the effect that variations in the Si/Al ratios, and applied those estimated to naturally-occurring systems. Our estimated values for $\Delta_f G^o_m$ of analcimes of composition $Na_{0.8}Al_{0.8}Si_{2.2}O_6 \cdot H_2O$ along with our experimental values for $Na_{0.96}Al_{0.96}Si_{2.04}O_6 \cdot H_2O$ suggest that solid solution of quartz in analcime is nearly ideal. These new Gibbs energies have been used to construct a log ${}_{SiO_2(aq)}$ against T phase diagram which depicts the stability of the analcimes with respect to quartz. This diagram is in complete harmony with geologic field observations and with the experimental determined stability limits of the analcimes.

In order to more completely understand the (heulandite-laumontite-SiO_2) and (heulandite-analcime-SiO_2) equilibria, our earlier studies on heulandite are being extended to include additional specimens with different Si-to-Al ratios.

Currently, the thermodynamic properties of mordenite and dehydrated mordenite are being determined in order, *inter alia*, to obtain a better understanding of the properties of zeolitic water.

Contractor: LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Contract: DE-AC03-76SF00098

Title: Geosciences Program

Person in Charge: T. V. McEvilly

Scope of Work

The geosciences program at LBL encompasses investigations in geochemistry, geophysics, reservoir dynamics, and applied geomechanics. In their applications, these studies are divided into five categories, represented in the following summaries: projects related to drilling for scientific purposes in thermal regimes on the continents, basic geochemical investigations, geomechanics-fracture studies, investigation of chemical and fluid transport processes, and the effects of bolide impacts on mass extinctions.

A. Continental Scientific Drilling - Related Projects

1. Hydrogeochemical Investigations (A. F. White and H. Wollenberg)

   The objective of the hydrogeochemical investigations is to evaluate active hydrothermal systems in the Long Valley and Valles calderas and the Salton Trough as potential targets for deep continental drilling into magma - hydrothermal regimes. The data derived are being used to determine to what extent chemical components are introduced into hydrothermal systems from deeper magmatic sources and to determine sources of meteoric water recharge and pathways of discharge. In cooperation with the U.S. Geological Survey, existing wells operated by geothermal companies have been sampled for major and trace fluid components and dissolved gases, including noble gas isotopes. Modeling of the chemical evolution of the systems is also under way using these data and reaction path geochemical codes. The project also provides geochemical and hydrogeologic support in the design of a downhole sampler for geothermal wells and the subsequent chemical analyses and their interpretation. The sampler system may be used in holes to be drilled by DOE in thermal regimes, beginning in 1984.

2. Deep Electromagnetic Sounding of the Crust (H. F. Morrison and N. E. Goldstein)

   Variations in electrical resistivity within the crust are related mainly to the degree of connected porosity, saturation and salinity of pore fluids, as well as past and present thermal effects; e.g., elevated temperatures and clays due to hydrothermal reactions. Interpreted with current thermal and seismic data, subsurface resistivities derived from electromagnetic soundings can yield important information on the source of thermal anomalies within the crust, including the possible location of shallow magma bodies.

Controlled-source EM (CSEM) soundings made in the Long Valley Caldera have delineated two apparently separate and distinct high conductivity areas at depths of 2.5 to 3 km and within pre-caldera rocks. One conductor occurs in the south moat and near the area of intense earthquake activity and presumed magma movement. It may be due to a combination of conductive rock within a Paleozoic roof pendant, high porosity due to fault-induced fractures, and elevated temperatures. The second conductor underlies the northeast corner of the resurgent dome and appears to plunge southeastward toward Lake Crowley. Because the conductor is concordant with a magnetic anomaly, there is the possibility that the conductor represents a post-caldera extensional zone intruded by mafic magnetic rocks. The presence of these conductors has raised new questions on caldera development and structure.

The 3-axis Superconducting Quantum Interference Detector (SQUID) magnetometers previously used with the CSEM system are being replaced by newly designed and built, lightweight induction coil magnetometers and matching amplifiers. Initial tests of the coils reveal that their intrinsic noise is as low or lower than the SQUIDs. The new magnetometers should result in lower operating and maintenance costs and be more reliable than the SQUIDs.

3. Center for Computational Seismology (T. V. McEvilly and E. L. Majer)

Seismology has traditionally been a data-intensive, multidisciplinary science with consequent problems in the reduction and analysis of large volumes of data on the one hand, and in the efficient handling, analysis, and presentation of results on the other. To be fully effective in seismology, a modern research laboratory requires data manipulation and storage capabilities beyond those of most computational facilities, along with a sophisticated flexibility in graphics and interactive operations.

It was apparent that existing personnel, equipment, and mutual interests at (UCB) and and Lawrence Berkeley Laboratory (LBL) provided a unique opportunity to establish the Center for Computational Seismology (CCS). The combined expertise in computer science, hardware development, data file management and manipulation, numerical analysis, computer graphics, and seismology offers a powerful center capability.

The basic LBL resources available to support CCS are the Computer Center and the Computer Science and Mathematics Department (CSAM). These resources can compensate for the hardware and software limitations discussed at the outset. The LBL Computer Center provides the basic computational equipment. This has the advantage of drawing upon the continuing hardware and software developments of a larger facility, thus minimizing the risk of obsolescence. We have added to these facilities the hardware and software necessary to run the seismic reflection imaging, and to provide the CCS user with terminal and graphics service. That is, we have established within a larger computational complex a specially equipped and staffed computational facility to support and advance the wide-ranging program of seismologic research and education within the UCB/LBL community.

The first year of operation has been devoted mainly to software development and utilization of the imaging package. The principal areas of research with our specific application are:

1. Deep reflection profiling techniques
    - San Andreas Fault
    - Charleston fault zone

2. Reflection profiling in thermal regions
    - Basin & Range (northern Nevada)
    - California Coast Range (The Geysers)
    - Salton Trough (Cerro Prieto)

3. Source mechanism studies
    - Long Valley microearthquake activity
    - The Geysers seismic activity
    - Coalinga earthquake sequence
    - Acoustic emission studies of thermally disturbed zones
    - Characterization of underground nuclear explosions

4. Wave propagation
    - Seismic tomography
    - Cross-hole seismic studies in basalt
    - Scattering and attenuation of seismic waves
    - Seismic polarization & signal enhancement
    - Surface wave studies across the Tibetan Plateau

5. Data base studies

Satellite data center for DARPA's Center for Seismic Studies
Regional data center for USGS Office of Global Seismology

In addition to the above research areas, CCS is interacting with Lawrence Livermore National Laboratory (LLNL) to provide facilities for reflection profiling processing for data acquired at the Nevada Test Site and to offer CCS as a host for the development of a VAX version of the LLNL seismic analysis code (SAC). CCS also became a member of the California Consortium for Crustal Studies (CALCRUST) initiative to the National Science Foundation for the processing, analysis, and archiving of reflection data in active western tectonic regions. In total, there is routine usage by seven graduate students, two postdoctoral research scientists, four faculty/LBL staff scientists and five undergraduates in geophysics or computer sciences. Visiting scientists came from LLNL(3), USGS, the State Seismological Bureau of the Peoples Republic of China, University of Washington, Penn State, and Cal State, Northridge.

4. Detailed Microearthquake Monitoring at the Long Valley Caldera (E. L. Majer and T. V. McEvilly)

The objective of the study is to determine the source mechanisms of the microearthquake activity inside the Long Valley Caldera compared with activity outside of the caldera. It has been postulated that much of the earthquake activity in this region may be due to magma intrusion. If so, the microearthquake activity may be an indication of the location of magma movement. A 15 and 12 station array of 3 component high frequency (4.5 hz) stations was deployed in successive 15 and 10 day studies in the south moat and Laurel Canyon areas, respectively, of the Long Valley Caldera. The data from the two separate arrays were telemetered to a central location and processed in real time with the Automated Seismic Processor (ASP). The results indicate that even at a detection threshold of $Mo = 10^{16}$ dyne-cm, the micro-earthquake activity is diffuse, with no clearly defined planes or clusters. All events detected were strike slip, consistent with regional tectonics. Events inside the caldera were deeper than those outside of the caldera, but no evidence was seen for a magma conduit.

B. Basic Geochemical Investigations

1. Thermodynamics of High-Temperatures Brines (K. S. Pitzer)

This project covers theoretical and experimental studies concerning the thermodynamic properties of aqueous electrolytes. The components important in natural waters and brines are emphasized. The resulting data are important in understanding certain geothermal and other natural resources. Moreover, this information has a wide range of applicability, since similar solutions arise in many industrial processes and in high-pressure steam power plants.

A theoretically based equation was developed for the thermodynamic properties of aqueous NaCl valid form 373-823 K, to 1 kbar, and to saturation with the solid. This extends to higher temperature the earlier treatment valid from 273-573 K.

The experimental program involves measuring the heat capacity and the density of solutions in the range 0 to 300°C and 0 to 1 kbar. These measurements suffice to give a comprehensive equation of state, provided that other thermodynamic properties are known for a particular system at room temperature and pressure.

Other recent theoretical work has yielded equations predicting the properties of mixtures based on the knowledge of the pure component solutions in water. In a number of cases, the calculated results for mixed brines are well verified by direct measurement. Phase equilibria can be predicted. Recent calculations have included solubility calculations of Na_2SO_4 and several alkali halides in a variety of mixed electrolytes usually to about 250°. Densities were measured recently for Na_2SO_4 and $MgSO_4$, and the heat capacity of the latter is now being measured. When these data are combined with earlier results, a comprehensive treatment can be given of phase equilibria over a range of temperatures for solutions containing the geochemically important ions Na^+, Mg^{+2}, Ca^{+2}, and Cl^-, SO_4^{-2}, HCO_3^-, OH^-, K^+.

2. Thermodynamic Properties of Silicate Liquids (I. S. E. Carmichael)

The objective of this program is to better understand the chemical and physical properties of silicate melts and their quench products, silicate glasses. These data see a wide range of applications, from the interpretation of the generation and evolution of natural magmas to the understanding of their molecular structure.

The ultrasonic velocity and attenuation of several dozen silicate liquids has been measured to obtain adiabatic compressibilities. Data have been collected on liquids with substantial amounts of all geologically major elements, as well as the alkali and alkaline earth oxides. Liquid and glass heat capacities of similarly wide compositional range, as well as heats of fusion of many silicates, have been measured calorimetricly. These results have been modeled to allow prediction of the properties of complex, multicomponent liquids, and to assess the average behavior (i.e., structural role) of each component.

Study of volatile solubilities in silicate melts has continued with work on both very inert (He, Ne, Ar, Kr, Xe) and chemically active gases (SO_3, O_2). Again, the results serve both to suggest underlying chemical mechanisms and to contribute to solving petrologic problems.

A highly sophisticated new drop calorimeter has been designed and is under construction. The instrument will be capable of operating to 2400°C with an accuracy of 0.1%, and will be used to measure heats of fusion and solid and liquid heat capacities for a wide range of very refractory and often geologically very abundant materials (i.e., Mg_2SiO_4). The high precision should permit the quantification of subtle effects which may have major physical significance, such as variation with temperature in heat capacity.

3. Generation and Migration of Petroleum and its Precursor Compounds (O. Weres)

The objective of this project is to study the reactions that produce hydrocarbons under conditions that resemble those under which petroleum is formed in nature. However, reactions are run at high temperature (usually 315°C) to allow reactions that require millions of years in nature to take place in days.

Experiments have been performed with oil shale, humic acid, synthetic models of kerogen (polymerized tung oil and terpene resins), and a variety of organic compounds. Present emphasis is on carboxylic acid anions. An important result is that large yields of acetate ion are obtained from a variety of starting materials, and that acetate ion is converted to methane. This supports the theory that the abundant acetate ion in oil- and gas field waters plays a major role in the formation of natural gas. The chemical behavior of other carboxylic acids, cycloketones, and the phenols under gas field conditions has also been investigated.

Results of this project have already found application in two disparate areas. Techniques developed by this project have been applied to analyzing a gas field brine from Texas, and helped explain why this brine was causing a serious environmental problem. The observation that humic acid yields a large amount of acetate at 315°C helped explain why acetate and similar species are the major anions in the condensate of nuclear powerplants. This is a major advance in the art and science of understanding and eliminating the chemical conditions that cause serious corrosion in many nuclear steam generators.

The use of propyl esters for the analysis of mixed carboxylic acids has been systematized, and a collection of propyl ester mass spectra will be published.

4. Rock-Water Interaction (J. A. Apps)

The objective of this project is to understand factors controlling albite solubility in aqueous solutions between 25°C and 400°C, and 0.1 to 50 MPa. The results permit refinement of rock-water interaction models. Presently, data from some 25 dissolution studies are being evaluated with the purpose of interpreting the thermodynamics and kinetics of albite dissolution in sodium chloride solutions over the temperature and pressure range specified.

5. Abiogenic Methane Production from Igneous and Metamorphic Rocks (J. A. Apps)

Hypotheses have recently been advanced in which it is asserted that large quantities of carbon remain trapped in the mantle after planetary accretion and differentiation, and that the progressive degassing of this carbon as methane may contribute to the world's oil and gas reserves. Petrological and geochemical arguments, however, infer that mantle degassing occurs primarily through release of carbon dioxide. Abiogenically produced methane may instead have a shallow, low temperature crustal origin due to hydrolysis by ultramafic and possibly mafic rocks.

Research is underway to determine, through theoretical and laboratory studies, the range of pressures, temperatures, and chemical conditions under which methane might form in igneous and metamorphic rocks during hydrolysis. Attention is being paid to the sources of carbon, and competing reactions involving sulfur and nitrogen.

6. Aqueous Solutions Database (S. L. Phillips)

The twofold objective of this project is the compilation of critically evaluated experimental data on selected equilibria in aqueous solutions to high temperatures, concentrations, and pressures; and, to publish tables of recommended values for these equilibrium quotients. The data are used, for example, in nuclear waste disposal, chemical oceanography, geothermal energy, hydrometallurgy and corrosion problems. However, emphasis is currently on nuclear waste disposal.

Besides chemical equilibria, data covered include electrode potentials, diffusion coefficients and adsorption. The basic data are used, for example, to predict solubility and speciation of radioelements in nuclear waste repositories that may be located in salt, basalt, and tuff. A result of this project is identification of gaps where data are lacking or are inadequate, and recommendations for research to provide the needed data.

Besides critical evaluation of data, research is included on calculation of stability constants to high temperatures and concentrations; as well as computerized storage and retrieval of tables of data using desktop computers.

C. Geomechanics/Fracture Studies

1. Effect of Fracture Characteristics Upon Sonic Wave Propagation in Boreholes (M. S. King)

Fluid flow in rock is governed by the product of a single rock parameter, permeability, and the hydrological potential gradient existing in the rock mass. The determination of permeability is critical to any endeavor for which a knowledge of fluid flow is required. Such fields of interest lie in geothermal energy extraction, oil and gas recovery, deep crustal studies, energy storage in aquifers, and the storage of hazardous wastes. In rocks of low porosity, including many igneous, metamorphic and massive calcareous types, the in situ permeability is controlled by the presence of fractures rather than by the rock matrix permeability.

Geophysical borehole methods are available for detecting the presence of fractures adjacent to a borehole and therefore potentially for assessing the rock mass permeability in those cases that it is controlled by fractures. In particular, the borehole sonic log has shown considerable promise for locating fractures in rock. Field experiments have been conducted in which digitized sonic log waveforms were obtained across single, horizontal, isolated fractures intersecting a borehole in a crystalline rock mass. The fluid flow characteristics of these isolated fractures were measured using conventional borehole packer techniques, and the results compared. The field test will be extended to zones in the same rock mass where systems of fractures intersect the borehole, and again the results of sonic and conventional packer tests will be compared. The theoretical aspects of elastic-wave propagation along a borehole intersecting a fracture or systems of fractures are also being studied, with a view to establishing the importance of fracture parameters such as aperture and roughness on acoustic velocity and attenuation. The field experiments and theoretical studies will be used to establish correlations between acoustic wave parameters and the permeability of the rock mass adjacent to the borehole.

2. Fundamental Studies of Fluid Flow in Fractured Rock Masses Under Stress (P. A. Witherspoon and Y. W. Tsang)

The objective of this research program is to gain a fundamental understanding of the factors governing fluid flow through a single rock fracture which is subject to stress. Understanding the fluid flow behavior in a single fracture is prerequisite to the determination of the permeability of fractured rock masses. This is of importance in many areas of practical interest such as the isolation of nuclear and toxic wastes, the recovery of fossil fuels, and the development of geothermal energy. Our theoretical studies show that the geometrical roughness of fracture surfaces holds the key to many hydromechanical properties which cannot be explained if fractures are assumed to be idealized, smooth, parallel plates. By incorporating fracture roughness, we find that: (1) the characteristic stress-strain curves for both well-mated and poorly-mated fractures can be derived, (2) the effect of sample size on the mechanical and hydraulic properties of the fracture are controlled by the large scale roughness of the fracture surfaces and (3) the tortuosity of flow paths may cause the fluid flow rate through the single fracture to be depressed by several orders of magnitude from values predicted from the parallel plate idealization.

D. Transport Processes

1. Nonisothermal Reservoir Dynamics (P. A. Witherspoon, C. F. Tsang, T. N. Narasimhan)

This project encompasses a wide range of fundamental studies of fluid, heat, and solute transport in underground formations. These studies are relevant to underground thermal energy storage, geological isolation of nuclear waste, chemical wastes disposal, and other energy-related projects. The goal is to better understand various physical and chemical transport processes in porous or fractured media and their effects through mathematical modeling and laboratory investigations.

Specifically, the following topics are addressed:

> Modeling of flows of heat, liquid, vapor and air through a fractured-porous medium. A computer code capable of calculating these processes is being developed. Applications are made to the study of non-isothermal unsaturated flow near an underground heating source.
>
> A new well test method to determine aquifer vertical permeability and layering characteristics. This proposed technique involves the injection of hotter or colder water into an aquifer and monitoring of the temperature variations. Field data are analyzed to validate the new method.
>
> Well test methods to characterize a fractured medium by means of coupled pressure, tracer, and thermal measurements.
>
> Continuation of the validation and applications of the LBL coupled thermo-hydromechanical code to model flow through fractured porous media.
>
> A new technique to improve grid orientation performance of a finite difference method with applications to pattern steam-flood problems.
>
> A study of the possibility of determining the shape and location of a fluid plume by means of coupled hydrologic and geophysical methods.

2. Chemical Transport in Natural Systems (C. L. Carnahan)

The objective of this research program is to better understand and characterize certain chemical and physical phenomena that influence the movement of chemically reactive solutes in groundwater flow systems. The results of the research are applicable, for example, to the migration of contaminants away from nuclear waste repositories and uranium mill tailings ponds, as well as to studies of geothermal energy reservoirs, hydro-thermal ore deposits, and other energy-related topics.

The principal focal point is the nonequilibrium nature of certain processes influential in chemical transport. Computer codes have been developed to study solute transport by advection and hydrodynamic dispersion in three-dimensional, axisymmetric flow systems in which chemical reactions occur between solutes and solid phases. Both linear, and nonlinear kinetic rate laws for these reactions have been used in the numerical models. The thermodynamics of irreversible processes is being used to describe coupled transport processes such as chemical osmosis, thermal osmosis, thermal diffusion, and ultrafiltration. Results obtained during 1983 show that certain coupled processes may be much more significant than previously realized in saturated geologic materials that behave as semi-permeable membranes. Such materials include clay-containing backfills for high-level nuclear waste repositories.

E. Bolide Impacts and Mass Extinctions (F. Asaro, W. Alvarez, and H. V. Michel)

The overall objective of this project is to determine the relationship between asteroidal or other large body impacts on the earth and repeated massive extinctions of life which have occurred in the last 570 million years (m.y.). The primary mechanism for the research consists of intensive chemical and selective mineralogical studies (on sediments near both major and minor extinction boundaries) which are run in parallel with floral and faunal fossil studies by collaborating geologists and paleontologists. A secondary but major objective is to ascertain if a series of time markers of very high precision and accuracy (in the form of iridium and other geochemical anomalies) can be developed for relative dating and correlation of sediments in many different parts of the world. A minor objective is to evaluate the major chemical and mineralogical alterations which have occurred in the sedimentation of the 65 m.y. old Cretaceous-Tertiary (K-T) boundary, the one most closely linked to a large body impact, in order to predict the behavior expected in older boundaries.

It has been shown by one of us (W.A.) in collaboration with Richard Muller of LBL that periodic extinctions, previously noted by others to occur in the fossil record every 26 m.y., are matched by a comparable periodicity in the ages of large well-dated craters on the earth. This match has given striking support and impetus to the new hypotheses which suggest the extinctions are related to comet showers originating in the outer fringes of the solar system. These showers could have been triggered periodically by a dark star orbiting the sun.

In studies with Miriam Kastner of U.C. San Diego of the mechanism of formation of the 65 m.y. old K-T boundary, it was found that the large bolide impact (which produced the anomalous iridium deposits) probably occurred on terrestrial basalt and that a homogenized mixture (10% bolide and 90% basalt) was distributed world-wide in the form of small glassy particles which altered to clay in the ensuing 65 m.y.

An exhaustive study was made of innovative new ways in which methods of x-ray fluorescence or neutron activation analysis could be economically and rapidly (i.e., within a few years) used to measure iridium concentrations continuously in 1 kilometer of sediment. X-ray fluorescence techniques appear fruitless but neutron activation analysis with new sophisticated electronic techniques of gamma-ray measurement is very practical. An Iridium Coincidence Spectrometer has been designed which will be capable of measuring iridium with high sensitivity in 100,000 samples per year at a reasonable cost and will permit a thorough search for iridium anomalies in sediments corresponding to the 26 m.y. periodicity found in the fossil and cratering records.

Contractor: LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California
Livermore, California 94550

Contract: W-7405-ENG-48

Title: I. Geology, Geophysics, and Earth Dynamics

Person in Charge: L. W. Younker

Scope of Work

The Geology, Geophysics, and Earth Dynamics Program at Lawrence Livermore National Laboratory consists of six projects: (A) Rock Mechanics, (B) Diffusion in Silicate Materials, (C) Electrical Conductivity and Temperature in Upper Mantle, (D) Attenuation and Dispersion in Rocks Containing Fluids, (E) Surface Wave Method for Determining Earthquake Mechanisms with Applications to Regional Stress Field Studies, and (F) Thermal Stress Microfracturing of Granite.

These research tasks are broadly based fundamental studies which have applications in a variety of areas including geothermal energy development, nuclear waste isolation, and seismic verification of nuclear test treaties.

A. Rock Mechanics (H. C. Heard, B. Bonner, and W. B. Durham)

This Laboratory program involves four related sub tasks:

Determination of the Thermal Behavior of Igneous Rocks. We are currently determining the thermal diffusivity of igneous rocks to 400°C and 200 MPa lithostatic pressure. For use primarily on relatively fine-grained rock samples of the order of 2.5 cm in diameter, the measurement technique produces precise and accurate measurements in a relatively short time, allowing detailed studies to be made of subtle variations of diffusivity with pressure and temperature and of variations from rock to rock. Five different igneous rock types are being measured.

Surface Topography of Rock Joints. The occurrence of large scale fractures in situ controls important rock mass properties, such as stiffness and permeability. We have constructed a computer controlled digital measurement apparatus for surface profiling along a traverse of 25 cm with vertical sensitivity of 25 μm in order to produce quantitative descriptions of these rough surfaces. Several crystalline igneous rock types are being profiled to test mathematical models of the joint closure process which indicate that surface topography is a critical parameter for prediction of both elasticity and fluid flow.

The Influence of Cation Impurities on Creep in Halite (salt). Since the design of high level waste repositories in salt can be expected to be strongly influenced by both depth and the maximum anticipated temperature, it is of vital importance to be able to predict accurately the closure rates of these underground workings. In nature, salt is usually very pure but occasionally exhibits important trace amounts of K^+, Mg^{+++}, and Ca^{++}. We have demonstrated that the steady-state flow rate in salt is dependent on stress, temperature, and impurity content. At impurity levels of 0.1 - 0.6% of K^+ or Mg^{++}, closure rates of repository workings may be 10^8 - 10^4 times slower at temperatures of 30 - 150°C in impure salt as compared to the pure material. These results are being extended to include effects of Ca^{++} and deformation history.

Elastic Behavior of Dolomite Single Crystals at High Temperature. We have undertaken an experiment to determine compressional and shear velocities in dolomite to 450°C and 400 MPa carbon dioxide pressure. The plastic flow stress in at least one direction of dolomite increases with temperature, and data relevant to the elastic constants should help us understand this anomalous behavior. Preliminary data show anisotropic increases of travel time, and demonstrate that the techniques developed for this work are viable.

B. Diffusion in Silicate Materials (F. J. Ryerson, W. B. Durham)

Oxygen diffusion in natural olivine (Fo_{92}) is being investigated as a function of temperature, oxygen fugacity, and orientation employing oxygen-18 enriched gas reservoirs. Profiles are analyzed by both ion microprobe and nuclear reaction techniques. The dependence of oxygen diffusivity upon oxygen fugacity will produce a more complete understanding of the defect chemistry as olivine. These results can also be correlated with data on the anelastic deformation of olivine, hopefully providing the mechanistic data which will allow confident extrapolation of high-strain rate data acquired in the laboratory to the low strain rate regimes characteristic of the crust and upper mantle. Future work will include the evaluation of pressure effects and other important rock-forming minerals.

C. Electrical Conductivity and Temperature in Upper Mantle (A. G. Duba) (Joint Project with T. J. Shankland at LANL)

The thermoelectric effect in the mantle minerals olivine and pyroxene is being measured as a function of temperature, orientation, oxygen fugacity, and iron content to investigate the effect of Mg/Si non-stoichiometry on mineral conductivity. The results apply to inference of upper mantle temperatures from electrical data. While there are seismic models to explain the low velocity zone (LVZ) as a solid-state phenomenon not requiring partial melting, the most well-constrained laboratory electrical measurements are more consistent with the partial melting hypothesis for the high conductivity layer (HCL) apparently associated with the LVZ. If the LVZ/HCL is not a partial melt layer, then mantle geotherms would be considerably lower than previously inferred on the basis of a partial melt zone under extensive regions of the earth. Hence, it is necessary, to better understand electrical conduction in mantle minerals, to find whether electrical data are a serious constraint on the low temperature geotherms suggested by solid state explanations of the LVZ. Data have been collected and are being analyzed for olivine from San Carlos Indian Reservation, Arizona and a synthetic forsterite.

D. Attenuation and Dispersion in Rocks Containing Fluids (J. G. Berryman, B. P. Bonner, R. C. Y. Chin, and G. W. Hedstrom)

The objective of this project is to combine theory and experiment to analyze attenuation and dispersion of elastic waves in partially or fully saturated rocks over a broad range of frequencies. The techniques developed in this work will be applicable to a broad range of basic problems in energy recovery, particularly hydrocarbon and geothermal exploration and resource assessment. The major accomplishments of this project so far include: (1) paper analyzing the dispersion of extensional waves in the experimentally important case of fluid-saturated porous cylinders, (2) two papers on new computational techniques, and very favorable comparison with experiments on pulse propagation and attenuation in fluid-saturated porous layers.

E. Surface Wave Method for Determining Earthquake Mechanisms with Applications to Regional Stress Field Studies (H. J. Patton and S. R. Taylor)

The primary purpose of this project is to use surface-wave excitation and seismic moment-tensor theories in order to obtain source mechanisms of remote western United States earthquakes. The source mechanisms will be used to study the state of stress in the northern Basic and Range and environs. Knowledge of the regional stress field and interpretations of sources of stress should aid in identifying areas of potential geothermal energy production and supply constraints for geophysical models of convective hydrothermal systems.

Start-up work has involved studies of the Q-structure of the Basin and Range and regionalization of surface-wave phase velocities in the western United States. In addition to elucidating the earth structure, our aim is to develop a capability to compute accurately the path transfer function for any epicentral path in the study area.

Regionalized Rayleigh- and Love-wave attenuation coefficients were measured across the Basin and Range province of western United States in the frequency range 0.02 - 0.2 Hz and were inverted simultaneously for shear-wave attenuation as a function of depth. The resulting shear-wave Z model is characterized by low Q_β in the lower crust ($Q_\beta \sim 100$) and Q_β decreasing in the upper mantle with lowest values ($Q_\beta \sim 30$) beneath 60 km depth. Our interpretation of these results is that the lithosphere is poorly developed beneath the Basin and Range and that the partially molten asthenosphere may reach very shallow depths, possibly to the base of the crust. This interpretation of the Q model, in conjunction with a geological and geophysical information, suggests that attenuation mechanisms involving partial melt predominate in the lower crust and upper mantle of the Basin and Range.

A compilation of single- and two-station phase velocity measurements for Love and Rayleigh waves in the 6-60 sec period range was used to study regional variations of phase velocities in the western United States. A tentative regionalization consisting of four major, geophysically distinct provinces and three lesser provinces can explain up to 40%-of the variation in Rayleigh-wave phase velocities and gives an RMS phase travel time error of 4-6 sec. The preliminary results are encouraging for the refinement of structural models of the lithosphere in major tectonic units of the western United States and for the capability to compute phase travel times accurately, a prerequisite for use of surface waves in source mechanism studies involving linear moment tensor inversion.

F. Thermal Stress Microfracturing of Granite (H. C. Heard, Joint project with H. F. Wang at the University of Wisconsin-Madison)

By applying a simple inclusion model, we are able to relate crack density to changes in either pressure or temperature. Comparison of these predictions for four igneous crystalline rocks with laboratory measurements of thermal expansion under pressure and bulk modulus at temperature indicate a good correlation. These initial results are being expanded to include characterization of microcrack porosities, as well as the distribution of microcrack shapes and closure pressures. The effect of pressure-temperature path dependence on physical properties will be determined directly by measurements of elastic wave velocities, electrical conductivity, and permeability. It is hoped that the microcrack data and model will provide an understanding of the physical property data.

Contractor: LAWRENCE LIVERMORE NATIONAL LABORATORY
University of California
Livermore, California 94550

Contract: W-7405-ENG-48

Title: II. Geochemistry

Person in Charge: L. W. Younker

Scope of Work

The Geochemistry Program at Lawrence Livermore National Laboratory consists of two projects: (A) Thermodynamic, Kinetics, and Transport in Aqueous Electrolyte Solutions, and (B) Kinetic and Compositional Model of High-Pressure Kerogen Pyrolysis. Studies include laboratory measurements of diffusion coefficients and activity coefficients for mixed salts, and kerogen pyrolysis experiments up to 1 kbar. Data obtained in the first task is important for understanding and modeling salt mixtures. The chemical kinetic model for kerogen conversion to petroleum as developed in the second task will have applications in a variety of fossil fuel programs.

A. Thermodynamics, Kinetics, and Transport in Aqueous Electrolyte Solutions (J. A. Rard and D. G. Miller)

Transport of dissolved chemical species is important in a wide variety of geochemical situations, including radioactive and chemical waste isolation, diagenesis, and ore formation. Mutual diffusion coefficient data are required to understand and model these processes. Osmotic and activity coefficient data are needed to model chemical equilibrium, including speciation and solubility. Some data are available for one electrolyte in water (a substantial fraction measured at LLNL). Much less data are available for two salts in water. Because such data are difficult to predict a priori, experimental measurements are esential. More activity data are available, but many mixtures of interest have not been studied. Accurate approximation methods need to be developed for mixtures to supplement all these data.

We have completed diffusion coefficient measurements for aqueous $MnCl_2$ (Rayleigh interferometry), and activity measurements for $MnCl_2$ and $MnSO_4$ (isopiestic method), since Mn^{2+} salts are of diagenetic interest. Diffusion measurements are complete for five NaCl-$SrCl_2$ compositions (waste isolation), and activity measurements are about 40% done for NaCl- $MgCl_2$ (seawater concentrates and brines), all at 25°C. These $NaCl-MgCl_2$ data extend to the crystallization limits.

B. Kinetic and Compositional Model of High-Pressure Kerogen Pyrolysis (A. K. Burnham)

The goal of this project is to link a chemical model for oil, gas, and water evolution that was derived from high pressure pyrolysis studies to the geological conditions present in the Uinta Basin. Various ways of interfacing the chemical model with the geology will be explored. The resulting calculations will be compared to observed deposits of oil and gas to understand more fully the mechanisms of oil formation and migration. The chemical model will be upgraded to more rigorously include the reactions of hydrogen so that H_2 and CH_4 production is more accurately calculated. Previous pyrolysis experiments will also be extended to variable porosity, hence variable residence time of the generated products in the pyrolysis region, in order to more fully decouple various mechanisms of oil degradation in the model. In addition, oil samples will be obtained and various biomarker ratios measured. Combined with analyses reported in the literature, these will provide further model verification when interpreted in terms of diagnostic trends establshied from analysis of oil samples produced in our laboratory at various conditions. This project will demonstrate how to effectively use laboratory pyrolysis experiments for other kerogens as an aid in both geochemical exploration and synthetic fuel production.

Contractor:	LAWRENCE LIVERMORE NATIONAL LABORATORY University of California Livermore, California 94550
Contract:	W-7405-ENG-48
Title:	III. Energy Resource Recognition, Evaluation and Utilization: Continental Scientific Drilling Program: Thermal Regimes
Person in Charge:	L. W. Younker

Scope of Work

The Continental Scientific Drilling Program at Lawrence Livermore National Laboratory consists of several projects, (A) Data Management, (B) Underground Imaging, (C) Viscosity Measurements, (D) Thermal and Petrologic Studies of Silicic Systems, (E) Information Base for the Imperial Valley, (F) Shallow Hole Drilling in the Long Valley, Valles, and Salton Sea Thermal Regimes, and (G) Seismic Studies of Possible Magma Injection and Magma Chambers in the Long Valley Region. These projects support the overall program in a variety of ways, including information and data management service, generic studies on site characterization techniques, generic studies on laboratory measurements of melt properties, studies of fossil analogue systems, thermal modeling of hydrothermal systems, and seismic characterization of target regions. In addition, a shallow research drilling program has been initiated at three thermal regime sites in cooperation with three other national laboratories (SNL, LANL, and LBL).

A. Continental Scientific Drilling Program Information and Data Management Unit (N. W. Howard)

Because of the extremely high cost of drilling, it is crucial that the geologic community be kept informed of the availability of drill holes and the data obtained from them. Numerous governmental agencies and research groups have drilled holes for a variety of purposes. In some cases, information has been disseminated on the availability of these holes for research purposes, and cooperative programs have been initiated between a number of academic, government, and industrial groups. More often, however, this information has not been disseminated and interested researchers have been unaware of the availability of these drill holes until it is too late to participate effectively. An information system has been established to avoid this problem. The efforts of a Continental Scientific Drilling Program (CSDP) can be expedited, unnecessary expenditures limited, and maximum data effectiveness attained by (1) utilization of pre-existing information; (2) reopening of abandoned holes; (3) participation in current industry drilling tests; and (4) participation in the drilling and study of future wells.

LLNL has developed a computerized data base for drill hole data acquired in CSDP projects, and is providing information to the scientific community on plans and drilling activities in a timely manner. It will continue to do so through the initial period of intensive use. A study of potential long-term operating modes has proved that there is still an active interest in the data base which is best served by having LLNL provide data compilations as requested by researchers.

B. Underground Imaging (R. J. Lytle and A. G. Duba)

A significant portion of the Department of Energy budget is being spent on extracting energy from, or storing nuclear waste within, the subsurface environment. To asses whether the energy extraction or waste storage procedures are properly implemented, it is necessary to obtain detailed images of the subsurface environment. Such images will also be of value for continental drilling interests. LLNL has had success in developing and applying the concept of geophysical tomography to achieve such images. LLNL has also shown that improved interpretations of the subsurface environment can be obtained by combining laboratory data on the relations between remote probing observables (such as seismic attenuation or electromagnetic velocity) and the governing physical phenomena (such as in situ stress of temperature). Demonstrations of seismic shear, seismic compressional and electromagnetic geotomography has been successfully completed. This effort will continue the integrated program for advancing the state-of-art in data collection methods, data processing procedures, data interpretation techniques, and enhanced means of data interpretation.

C. Viscosity and Liquid Lines of Descent for Rock Melts: Continental Scientific Drilling Program (H. C. Weed, F. J. Ryerson, and A. J. Piwinskii)

Viscosities and liquid lines of descent are being determined for molten silicates under conditions of controlled oxygen fugacity (QFM). These data will relate rheological properties to the percentage of suspended crystals in a magma, and should be of value in understanding mass and thermal transport in petrologic phenomena. Materials currently under evaluation include primitive tholeiitic and high-Al basalts from Kilauea Iki and the Medicine Lake Highlands. The results should be applicable to targets selected for deep continental drilling.

D. Thermal and Petrologic Studies of Large Silicic Systems (L. W. Younker, P. W. Kasameyer, and T. A. Vogel (Michigan State University))

An important aspect of continental crustal evolution is the injection into the upper crust of magma from the upper mantle or lower crust and subsequent modification of the crust as a result of thermal energy and volatiles released from the magma. The thermal regimes portion of the Continental Scientific Drilling Program (CSDP) seeks to understand these processes which involve development of geothermal systems, mineral deposits and volcanism through direct observation of the magmatic and near magmatic environment.

Our support for this CSDP initiative falls roughly into two categories (1) geological and geochemical field studies of selected exhumed fossil magma systems, and (2) thermal modeling of the shallow hydrothermal system at the Salton Sea Geothermal.

Exhumed Fossil Magma Systems. We have undertaken an integrated program of field and laboratory studies of the volcanic eruptions from two major volcanic systems in southern Nevada. The southern Nevada volcanic field of middle to late Miocene age is one of the most intensely studied and best understood fields in the world. Work, largely by geologists of the U.S. Geological Survey, has lead to the identification of more than twenty major ash-flow sheets and at least eight collapse calderas. These major volcanic eruptions provide a large instantaneous inverted sample of the subsurface magma body, and as a result, provide an excellent opportunity to study the evolution of high-level silicic magma systems. We have to date focused on the Black Mountain volcanic system for a detailed geological, geochemical and petrological study. We have complemented that study with an analysis of one of the major eruptions from the Timber Mountain Caldera complex. The results of the study have provided us with information on how these crustal magmas evolve and the dynamics of major volcanic eruptions.

Salton Sea Geothermal Field. The Salton Sea Geothermal System, a hot hypersaline convecting system driven by intrusions into a sediment-smothered rift system north of the Gulf of California, has been recognized as one place where magmatic/hydrothermal processes can be observed and analyzed. Modeling of the hydrothermal system based on thermal and geophysical data has enabled us to put constraints on the rate of magma intrusion, the timing of the initiation of the most recent hydrothermal system, and the associated flow pathways and rates. It is expected that future dedicated drilling at this site will help to further resolve the relationship between the magma intrusions and the surrounding hydrothermal system.

E. CSDP: Imperial Valley Information Base (D. O. Emerson and P. W. Kasameyer)

To assist the CSDP-Thermal Regimes Program select sites for additional studies and determine the types of research that are needed, an information base is being developed for the Salton Trough. The data base will contain standard bibliographic data that can be searched using keywords, lists of researchers who are currently engaged in research in the area with a brief summary of their interests, and a generalized plan for future research, including possible drilling project. Using a conventional commercial data base management system on IBM-PC computers, this data will be distributed in printed form on a semi-annual basis with the first set being available September 1, 1984.

F. Shallow Hole Investigation of Long Valley, Valles, and Salton Sea Thermal Regimes (L. W. Younker, P. W. Kasameyer, and J. F. Scheimer) (Cooperative program with SNL, LANL, and LBL)

The intrusion of magma into the upper crust, the release of heat and volatiles from these intrusions, and the development of associated hydrothermal systems are problems central to understanding the evolution of continental crust and its resources. Recent research into magma/hydrothermal systems under the Continental Scientific Drilling Program have concentrated on Long Valley Valles Caldera, and the Salton Sea. All three areas contain major, recently active magmatic systems and currently active hydrothermal systems. A general reconnaissance phase of work is well advanced at these sites, and has defined specific questions which can be addressed by shallow drilling. These questions involve the mechanical, chemical (particularly with respect to volatiles), and thermal behavior of magma at shallow depth, and the the composition and circulation pattern of hydrothermal fluids. An interdisciplinary and interlaboratory program of investigations in shallow holes is proposed for the three candidate Continental Drilling sites, as a necessary step toward deep drilling at these sites. Drilling targets are the conduits beneath the youngest vents at Long Valley and Valles Calderas, and an unexplored region of the Salton Sea thermal anomaly.

LLNL involvement in the project will concentrate on thermal model development, geophysical characterization of the sites and petrological support. At Banco Bonito, we will use borehole geophysics to define the geometry of the vent structure. In addition, monitoring of the response of pore pressure to tidal strain will allow us to characterize the orientation of the major fractures, encountered in the well. Combined interpretation of these two sets of data would provide constraints on the nature of the ring fracture system. At the Salton Sea, we will plan the heat flow survey, select the subcontractor and interpret the data using a recently developed model. We will use the new data and the refined model to provide new constraints on the volume, density, and location of the igneous dikes which provide the heat to the system.

G. Seismic Studies of Possible Magma Injection and Magma Chambers in the Long Valley Region (J. M. Mills, A. T. Smith, and J. F. Scheimer)

Our seismic research program in Long Valley/Mono Craters area emphasizes two approaches:

High resolution seismic studies to determine mechanisms of possible magma injection.

Crustal structure studies to locate and define a possible magma chamber.

Data collected in August 1982 and August 1983 in cooperation with a number of other agencies, including the USGS, provides the basis for the analysis.

Subtask 1: High resolution seismic studies of possible magmatic intrusion. The basic analysis will be extended from a single swarm to the remainder of the high-resolution data set. In addition, more advanced analysis of the entire data using source and attenuation models will enable us to further constrain the mechanics of the apparent injection process.

Subtask 2: P and S wave crustal structure studies. We will analyze the existing 3-component seismic data from the timed explosions and earthquakes using 2-D and 3-D inversion techniques, and applying 2-D forward modeling techniques. Modeling converted phases already identified in the seismic records may determine if they are produced at a solid-rock/magma interface. The Q_{coda} method of Aki will also be used to determine if ray paths through proposed regions of magma show anomalously high shear wave attentuation.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: I. Geophysics

Person in Charge: J. T. Whetten

Scope of Work

Geophysics research at Los Alamos National Laboratory presently consists of three subtasks: (A) Electrical Conductivity and Radiative Transport in the Earth; (B) Nonlinear Generation of Acoustic Beams; and (C) Creep Deformation of Rock. These research tasks apply importantly to technology needs in waste isolation and geothermal energy.

A. Electrical Conductivity and Radiative Transport in the Earth (T. J. Shankland and A. G. Duba (Lawrence Livermore National Laboratory))

We are measuring the thermoelectric effect in the mantle minerals olivine and pyroxene as a function of temperature, orientation, oxygen fugacity, and iron content and are investigating the effect of magnesium/silicon nonstoichiometry on mineral conductivity from radiative heat transport in a variety of materials that figure in geothermal studies, nuclear waste isolation, and solid-earth geophysics. The results of both of these efforts apply to inferences of the temperature distribution in the upper mantle and lower crust of the earth.

Because temperature differences in the earth drive tectonic motions on the earth's surface and interior, improved knowledge of thermal patterns is a requirement for evaluating seismic and volcanic hazards. Further, knowledge of the thermal state of the crust and upper mantle is essential for regional geothermal prospecting, particularly for the Continental Scientific Drilling Program.

B. Nonlinear Generation of Acoustic Beams (T. J. Shankland and J. N. Albright)

We are using the nonlinear elastic properties of rocks to generate low-frequency, long-wavelength acoustic beams in analogy with the case in laser optics. Two narrow beams of high-frequency sound can interact in a nonlinear medium to produce a narrow beam at their much lower difference frequency. The lower frequency beam has the narrow width of the generating beams, but it can travel much farther because of lower attenuation. Such a narrow beam would permit examination of acoustic interfaces from mine interiors and wellbores without the ambiguities of conventional seismology that use undirected sources, for example, transducers or explosives that broadcast energy in an almost spherical pattern. Should beam formation prove possible, there would be numerous applications to problems such as mapping fractures, the boundaries of ore and coal bodies, burn fronts in underground retorts, and fluid locations in oil, gas, and geothermal reservoirs. Of more interest to basic research in rock physics is the investigation of nonlinear properties of rocks and frequency dependence of elastic properties.

Nonlinear acoustic beams have previously been observed in homogeneous materials and fluids; however, rocks have the advantage of much greater nonlinear coefficients owing to the strong effect of crack closure on elastic properties. In preliminary results we have observed difference frequency generation from vibroseis transducers operating in the field and from piezoelectric transducers on laboratory specimens at high frequencies.

C. Creep Deformation of Rock (J. D. Blacic)

Assurance of long-term isolation of nuclear wastes in mined cavities in hard rock requires knowledge of time-dependent strength and transport properties of these rocks. Normal, short-time engineering tests do not encompass the full effects of phenomena such as water-aided stress corrosion and hydrolytic weakening. Therefore, we study creep deformation of basalt, granite, and tuff at simulated in situ conditions of temperature, pressure, pore pressure, and differential stress. Emphasis is placed on evaluating effects of water on time-dependent brittle deformation of intact vs. fractured samples and the effect of creep on fluid permeability. Results of the experiments will be formulated into creep constitutive relations in a form amenable to predictive computer models of repository designs.

Contractor: LOS ALAMOS NATIONAL LABORATORY
University of California
Los Alamos, New Mexico 87545

Contract: W-7405-ENG-36

Title: II. Geochemistry

Person in Charge: R. W. Charles

Scope of Work

Geochemistry research consists of eight subtasks: (A) Rock-Water Interactions in the Jemez Geothermal System; (B) Element Migration and Fixation in Rocks; (C) Physicochemical Basis of the Na-K-Ca Geothermomemter; (D) Cation Site Size and Coulomb Energy Calculations for the Principal Rock-Forming Minerals; (E) Coal Maturation: Occurrence, Form, and Distribution of Sulfur and Mineral Matter in Peat; (F) Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures; (G) Geochemistry of Technetium and Ruthenium and Geochemical Controls on the Redistribution of Multivalent Elements in the Lithosphere; and (H) Geologic, Geochemical, and Sr, Nd, and Pb Isotopic Studies on the Anomalous Late Cenozoic Basalt Province in the Southwestern Great Basin.

A. Rock-Water Interactions in the Jemez Hydrothermal System (R. W. Charles, R. J. Vidale, and F. Goff)

Experimental and theoretical studies are coordinated with field work to investigate rock-water interactions in the Jemez geothermal system, Northcentral New Mexico. The Jemez hydrothermal system includes at least three major hot circulating aqueous fluids, each of which has a characteristic major and minor element chemistry and is associated with characteristic rock alteration. Experimental studies will be coordinated with field work in order to define the principal variables as the system changes or has changed with time.

The approach is to define the stable mineral assemblages for a given set of variables by equilibration in agitated and, later, in circulating systems. Thermodynamic calculations will help fix these mineral assemblages in $f(O_2)$, $f(CO_2)$, $f(S_2)$, and pH space and, if thermodynamic data is not available, in chemical potential space. The experimental observations allow us to interpret the occurrence of natural alterations in portions of the Jemez system and to model the progress of such alteration through time, especially, in relation to known and proto-ore deposits.

B. Element Migration and Fixation in Crustal Rocks (T. M. Benjamin, R. W. Charles, and G.K. Bayhurst)

Acquiring an understanding of trace element migration and fixation in rocks requires a multifaceted experimental effort. Studies include: 1) the determination of the trace element concentrations and distribution in discrete mineral phases; (2) the conditions and mechanisms of element mobilization; and 3) the incorporation in secondary, precipitated, phases. Determining the major element compositions and spatial distributions in the solid phases utilizes well known electron microprobe and scanning electron microscopy techniques. The trace elements analyses are obtained from improved instrumental neutron activation analysis of bulk samples and our newly developed nuclear microprobe. The nuclear microprobe uses MeV energy protons, focused to micron size spots by a super conducting solenoid final lens, to yield characteristic x-rays resulting in elemental sensitivities, in favorable circumstances, in the 5 ppm range. The hydrothermal experiments are conducted in static Dickson vessels and dynamic fixed temperature circulating systems. The rock-aqueous fluid equilibration experiments are run at controlled pressure, temperature, and complexing anion composition. Solution samples are obtained at pressure and temperature allowing the experimental run to continue uninterrupted while obtaining unfractionated aqueous fluid. These solutions are analyzed by ion chromatography and plasma emission spectrometry.

This work can be used to examine economic recovery of metals in a geothermal energy extraction system, the origin of ore bodies, and the behavior of elements in a hazardous waste repository.

C. Physicochemical Basis of the Na-K-Ca Geothermometer (T. M. Benjamin, W. R. Charles, and G. K. Bayhurst)

The Na-K-Ca geothermometer uses these cation concentrations in the emergent aqueous fluid from geothermal systems to deduce the temperature of equilibration of the subterranean hot rock and coexisting fluid. Fournier and Truesdell (USGS) utilized surface water samples and temperature measurements to derive empirical constants for a feldspar controlled system. This form of the Na-K-Ca geothermometer has been successfully applied, with limitations, to many reservoirs and has undergone some modification to take into account, where necessary, other elements in the solutions.

A series of experiments is underway to address the two primary limitations of the empirical geothermometer, temperature calibration and the chemical basis of the geothermometer. Temperature calibration is required because although the solution cation concentrations tend to preserve the highest temperature of equilibration the emergent fluid may be significantly cooler so that the empirical geothermometer will yield temperatures below the true temperature of equilibration. The physicochemical basis needs to be understood so that the applicability of a given geothermometer, or which of a series of distinct geothermometer formulations, are appropriate in a given geochemical setting. We have observed that the activities of Na-K-Ca are fixed by secondary phases produced by reaction of the feldspars (± quartz) with water. Characterization of these secondary overgrowth is the thrust of the experimentation. Because granites provide the thermal source in many geothermal systems, granite plus aqueous fluid (± complexing anions) is reacted in both static Dickson and dynamic circulating systems.

D. Cation Site Size and Coulomb Energy Calculations for the Principal Rock-Forming Minerals (J. R. Smyth)

We will compile published crystallographic data on ordered end-members of the principal mineral groups and common accessory phases in igneous and metamorphic rocks and calculate from these, mean bond distances, volumes and distortion indices or coordination polyhedra, and coulomb potentials for all cation sites. This research will result in a reference publication that will facilitate understanding of inter- and intracrystalline major and trace element fractionation trends, recognize effects of some accessory phases on whole-rock trace-element distributions, and facilitate understanding of intracrystalline diffusion kinetics and chemical effects on mineral compressibilities. Data allowing us to interpret these important phenomena are not presently available for most mineral groups.

Computer program development and modification are largely completed, and data compilation is completed. Loading of crystallographic data onto computer disk files has been completed. We will continue our calculation and correlations of cation site sizes and coulomb potentials to observed inter- and intracrystalline fractionation trends, and we intend to collect our data in a reference publication.

E. Coal Maturation: Occurrence, Form, and Distribution of Sulfur and Mineral Matter in Peat (R. Raymond, Jr. and A. D. Cohen)

Elemental, mineralogic, and petrographic compositions of peats, the precursors of coals, are controlled by a combination of botanical and depositional environments. Diagenetic alterations occur within these various environments that will eventually affect the occurrence of sulfur and/or mineral matter in coal deposits. To evaluate the occurrence of sulfur and/or mineral matter in a coal deposit, one must understand the mechanisms for the introduction into the original peat deposit and the alterations they go through during stages of peatification.

We are investigating sulfur and mineral matter emplacement, distribution, and alteration in four distinct coal-forming regions: marine to brackish water environments (Everglades, SW Florida); salt marsh/freshwater complex (Snuggedy Swamp, South Carolina); freshwater swamp-march complex (Okefenokee Swamp, Georgia); and a freshwater complex with late stage marine incursion (Cranberry Island, Maine). The objectives of our research are: (1) to identify and correlate sulfur forms, authigenic minerals, and detrital minerals found in different peat types; (2) to identify the processes that enhance and/or inhibit distribution and preservation of sulfur and mineral matter in the initial coal-forming environment; and (3) to construct geochemical models for their formation, preservation, alteration, and distributuion based on the first two objectives.

Our approach is to use scanning electron microscopy, x-ray diffraction, fluorescent, and plain optical microscopy, bulk chemical analyses, and conventional sedimentological analyses to characterize the modes of occurrence and content of both sulfur forms and biogenically and non-biogenically derived mineral matter in peat types. We will thereby be able to establish relationships between sulfur and mineral matter occurrence and peat types, and also to correlate the concentration and forms of their occurrence with specific environments of deposition.

F. Thermodynamic Properties of Aqueous Solutions at High Temperatures and Pressures (P. S. Z. Rogers and C. E. Holley)

Knowledge of the thermodynamic properties of aqueous solutions is basic to an understanding of many geochemical systems. Hydrothermal alteration, element migration, and geothermal activity, are a few examples of processes largely dependent on the properties of the associated aqueous fluid. Studies of these processes require information on the heat content and ion activities of mixed electrolyte solutions over a wide range of composition and temperature.

Construction of a flow microcalorimeter, designed to measure the heat capacities of aqueous solutions, has recently been completed. The calorimeter has several features that make it a unique and powerful tool for determining the properties of electrolyte solutions. The most important of these is that the fluid flows through the calorimeter, allowing measurements along isobars (rather than along the saturated vapor pressure curve) and allowing sample changes without disturbing the temperature equilibration of the calorimeter. All parts of the calorimeter that contact the aqueous solutions are constructed of a special platinum alloy, providing corrosion resistance over the operating temperature range of 25°C to 350°C. The calorimeter also has been completely automated for nearly continuous operation.

The number of different electrolyte solutions of interest at high temperatures is large, so a method of obtaining thermodynamic properties from a minimum amount of experimental data is desirable. Heat-capacity measurements are ideal for this purpose because the heat capacity data can be integrated as a function of temperature to determine solution enthalpies and the ion activities of solution species. These thermodynamic properties will be used to provide an accurate model for electrolyte solutions at high temperature and pressures.

G. The Geochemistry of Technetium and Ruthenium and Geochemical Controls on the Redistribution of Multivalent Elements in the Lithosphere (D. B. Curtis, R. E. Perrin, D. J. Rokop, and K. Daniels)

Methods of isotope geochemistry provide powerful tools for studying the alteration of rocks: nuclear processes change the chemical and isotopic composition of natural materials in situ. The relative abundance of these natural nuclear products in a chemically isolated system can be predicted, usually by rather straightforward models of the nuclear processes. Discrepancies between predicted and actual abundances manifest the effects of chemical processes in the lithic environment.

Commonly these methods involve radioactive nuclides and their decay products (^{238}U-^{234}U, ^{87}Rb-^{87}Sr). However, the number of chemical elements represented by radioactive parent-daughter pairs is limited. In contrast, spontaneous fission produces nuclides that represent roughly one third of all the elements on the periodic table. However, the rate of element production by this process is so slow, the rate constant is 8.5×10^{17}/year, that the quantities of most elements produced in the entire history of the earth are imperceptible relative to those found "naturally" in geologic materials. In the case of a few elements, the "natural" component is sufficiently small that the spontaneous fission product can be detected. Ruthenium and technetium are two such elements. Because the abundances of these spontaneous fission products are so small there have been few efforts to develop the sophisticated analytical techniques and information required to use them as geochemical tools. We are using the unique capabilities of the Los Alamos National Laboratory Isotope Geochemistry Group to make the measurements. The ability to do so permits us to address several matters of importance. Both ruthenium and technetium are multivalent elements. Studies of their stability will provide information about the effects of redox conditions on the long term retention of multivalent elements in a geologic environment. Our work is one of the first attempts to explicitly examine the geochemistry of this rare element. Ruthenium is one of six geochemically similar elements termed platinum group metals. Some of these are important components of critical industrial processes. Studies of the geochemistry of ruthenium will contribute to our understanding of processes that enrich platinum group metals and thus enhance the ability to assess the reserves of these critical resources.

H. Geologic, Geochemical and Sr, Nd, and Pb Isotopic Studies on an Anomalous Late Cenozoic Basalt Province in the Southwestern Great Basin (B. M. Crowe, D. B. Curtis, and G. L. Farmer)

Field investigations are being undertaken to study the age, and geochemical and isotopic patterns of basaltic volcanism in a narrow strip extending from the western edge of the Nevada Test Site westward to the eastern edge of the Sierra Nevada range. This strip crosses several major structural features including: 1) the Death Valley-Pancake Range volcanic zone; 2) the western edge of the North American craton; and 3) an east-to-west transition in the degree of activity of basin-range tectonism. Associated with these structural features are: 1) a petrological transition in the composition of basaltic rocks from hawaiites to potassium-rich alkali basalts; and 2) a transition in the isotopic composition of neodymium and strontium ranging from mantle array basalts (Sierra Nevada edge) to highly anomalous basalts (Nevada Test Site region). Lead isotopic data for basalts are available only for the eastern and western edges of the strip. These data define a linear array on a $^{207}/^{206}Pb$ versus $^{204}/^{206}Pb$ diagram indicating a common aspect to the geochemical history of the rocks. The lead isotopic compositions of individual samples does not show a recognizable covariance with the neodymium-strontium isotopic composition , with variations in trace element contents or with geographic location of the studies basalts. It is not presently known whether differences in the lead isotopic composition of the basalts reflect a heterogeneous source region or differing degrees of contamination. Selected basalts, rhyolites, and Cretaceous granites will be mapped and sampled in the field and analyzed for age, major and trace element chemistry, and the isotopic composition of lead, neodymium, and strontium. The primary thrusts of the work are: 1) To determine if isotopic covariation exists between the basalts and crustal rocks and if such covariation is consistent with models of crustal contamination; 2) To attempt to relate the isotopic compositions of lead to strontium and neodymium isotopic variations for the basalts, the rhyolites, and the granites; and 3) To attempt to related the lead isotopic compositions of studied basalts to lead isotopic data for basalts from larger region of the southwestern United States.

Contractor:	LOS ALAMOS NATIONAL LABORATORY University of California Los Alamos, New Mexico 87545
Contract:	W-7405-ENG-36
Title:	III. Thermal Regimes and Continental Scientific Drilling Program
Person in Charge:	J. T. Whetten

Scope of Work

Research in Thermal Regimes and the Continental Scientific Drilling Program at Los Alamos National Laboratory consists of four items: (A) Studies of the Polvadera Group; (B) Origin and Extent of the Toledo Caldera; (C) Anomalous Lithospheric Structure Beneath Valles Caldera; (D) Shallow Hole Investigation of Long Valley, Valles, and Salton Sea Thermal Regimes; and (E) Valles Caldera Information Base.

A. Field, Petrologic, and Geochemical Studies of the Polvadera Group, Jemez Mountains, New Mexico (W. S. Baldridge and D. T. Vaniman)

The Polvadera Group consists of basalts, andesites, dacites, and rhyolites erupted between 10 and 2 m.y. ago on the northern, northeastern and eastern sides of the Jemez volcanic field. Basalts, comprising the Lobato Formation, were erupted earliest during Polvadera volcanism--between 10 and 7 m.y. ago. They range in composition, but at least two distinct groups are present based in both major- and minor-element characteristics. Field relations in the Lobato are complex, possibly indicating that systematic differences in composition occurred with time, or perhaps that different vents erupted different compositions simultaneously. Detailed mapping is underway to resolve these chemical-stratigraphic relations.

Andesitic and dacitic lavas (Tschicoma Formation) occur both as domes and flows. Dome distributions are being studied to the north and east of the Toledo caldera, where extensive vertical sections are exposed. Forth new chemical analyses are helping to define variability within and between the Tschicoma domes and flows to examine magma chamber processes.

Rhyolitic lavas (El Rechuelos Formation) were erupted late in the Polvadera cycle. These lavas may be early derivaties from a magma parental to the Valles (Bandelier) eruptions, or they may have oeveloped by parallel processes from other magma sources. New potassium-argon ages are currently being obtained to constrain stratigraphic relations within the Polvadera Group.

This work will lead to a more complete understanding of the magma chamber or chambers active 2-10 m.y. ago, of processes governing changes in magma compositions, and of the overall petrogenetic history of the Jemez volcanic field. It will also lead to an understanding of the ages, forms, and volumes of volcanic constructs that border the Valles caldera, and thus, will be important in interpreting results obtained in Continental Scientific Drilling Program drill studies.

B. Origin and Extent of the Toledo Caldera, Jemez Mountain, New Mexico, and its Relation to the Valles Caldera (G. H. Heiken and F. E. Goff)

The Toledo caldera is the older of two large calderas formed during the eruption of upper and lower members of the Bandelier Tuff. It is a major volcanic structure within the Jemez Mountains volcanic field, New Mexico, but its location and extent is poorly understood because much of the caldera has been masked by overlap of the younger Valles caldera. If a borehole is to be drilled by the Continental Scientific Drilling Program within the caldera complex, one option would be to choose a drill site located within the overlap of both calderas; this will provide maximum information on their history, structure, and geothermal systems. To this we must learn the extent and original position of the Toledo caldera. We propose to locate the buried portions of the Toledo caldera through geochronologic, stratigraphic, and petrologic study of domes, pyroclastic and sedimentary deposits located within the exposed remnant of the Toledo caldera, along the northern edge of Valles caldera and along the eastern flanks of the caldera complex, where the tuffs are interbedded between the upper an lower members of the Bandelier Tuff. These data should provide information on source areas for these deposits within the Toldeo caldera and, indirectly, its original location and extent.

We have nearly completed geologic mapping of most of the domes, tuffs, and sediments of the Cerro Toledo Rhyolite at a scale of 1:24,000. We have identified six eruption sequences within the Cerro Toledo Rhyolite. All consist of rhyolitic tephra and most contain Plinian pumice-falls and thin beds of very fine-grained ash of phreatomagmatic origin. Most Toledo deposits are thickest in paleocanyons and generally absent on pre-upper Bandelier ridges. Some of the phreatomagmatic tuffs flowed down canyons from the caldera and were deposited as base surges.

The tuffs are limited to two zones: 1) a 200-km-wide band that trends E to NE of the Toledo caldera (from the north edge of the Valle Grande to the north rim of the Toledo caldera); and 2) a SE-trending, 4-km-wide tuff blanket from Rabbit Mountain. There are no Cerro Toledo tuffs exposed elsewhere around the Jemez Mountains.

All of the major tuff sequences from Toledo intracaldera activity are separated by epiclastic sediments that represent periods of erosion and deposition in channels.

A study of the gravity data and drillhole data indicates that caldera resurgence is not reflected in the basement structure below Redondo Peak. On the basis of these observations, we are now evaluating models of resurgence associated with the Jemez caldera complex.

C. Lithospheric Structure and Volcanotectonic Evolution Beneath the Jemez Mountains and Rio Grande Rift Using Techniques of Seismic Tomography (K. H. Olsen)

The objective of this project is to investigate lateral variations in earth structure and rock properties (elastic wave velocities, densities, inferred temperature, etc.) beneath a complex volcanotectonic regime in northern New Mexico. We employ mainly geophysical techniques to characterize earth structure from depths of about 1-2 km to the level of the Mohorovicic discontinuity (approximately 35 km), which are beyond access by conventional surface geological techniques, although we incorporate geological and geochemical data by other investigators in our interpretations.

Our principal techniques are seismic: 1) time delay and synthetic modeling of amplitudes and waveforms of seismic waves from local and regional sources (mainly explosions); 2) merged common-depth-point (CDP) reflection and wide-angle-refraction profiling for high-resolution studies of stratigraphy of near-surface (less than 5 km) layers; and 3) time-delay observations from teleseismic (distances beyond 2000 km) sources, which are best suited for delineating mantle-level anomalies at comparatively low resolution. We combine these seismic data with gravity, aeromagnetic, and local earthquake location data derived from other Los Alamos programs to form an integrated geophysical picture of the study area.

This study deals, in general, with broad tectonic and evolutionary questions concerning the Rio Grande rift, one of the major active continental rift systems of the world. However, the principal focus of this ongoing study since 1981 has been the Jemez Mountain Volcanic Zone, which is one of the keystone elements of the rift. The Jemez region is a 100-km x 100-km x 50-km-deep block of the earth's crust that will be intensively studied using many geoscience disciplines (including deep research drilling) during the coming decade in order to clarify fundamental scientific questions pertaining to structure and evolution of large volcanic complexes and related hydrothermal geothermal systems.

D. Shallow Hole Investigation of Long Valley, Valles, and Salton Sea Thermal Regimes (F. E. Goff and J. C. Rowley)

The intrusion of magma into the upper crust, the release of heat and volatiles from these intrusions, and the development of associated hydrothermal systems are problems central to understanding the evolution of continental crust and its resources. Recent research into magma/hydrothermal systems under the continental Scientific Drilling Program (CSDP) has concentrated on Long Valley caldera, Valles caldera, and the Salton Sea. All three areas contain major, recently active magmatic systems and currently active hydrothermal systems. An interdisciplinary and interlaboratory program of investigations in shallow holes is underway for the three candidate CSDP sites as a necessary step toward deep drilling at these sites. Drilling targets are the youngest volcanic vents at Long Valley and Valles caldera and an unexplored region of the Salton Sea thermal anomaly.

Los Alamos has begun the contracting and coordination activities necessary to core a 650-m-deep hole down the Banco Bonito vent. Various geophysical logs will be obtained from the well during the later part of FY84. Strain rates will be measured on cores at Valles and on those obtained from Long Valley. Los Alamos is conducting petrologic studies of phenocryst phases as functions of depth in the rhyolite cores from the two sites and will continue with these investigations during FY85. Hydrologic tests will be performed on several aquifers of interest in the Banco Bonito corehole during FY85. Investigations of aquifer geochemistry and hydrothermal alterations will be conducted in collaboration with the other laboratories in order to help determine the characteristics of hydrothermal systems in the ring-fracture zone of Valles. Los Alamos will coordinate additional scientific efforts in the Valles corehole by the other laboratories and other interested research groups.

E. Valles Caldera Information Base (N. Marusak and F. Goff)

This is a continuation of an integrated information base containing references to published geologic, geophysical, and geochemical data and interpretations for considering detailed site selection for CSDP-Thermal Regimes. This task involves coordination with LLNL and Sandia with the objective of selecting a conventional commercial data base management system and compatible computer hardware for this project. Los Alamos has selected appropriate bibliographic titles for the assigned task from the Georef data base and DOE Energy data base. We have received these titles on tapes and are in the process of loading them into the computer for producing the hard copy listing of references.

Contractor:	LOS ALAMOS NATIONAL LABORATORY University of California Lcs Alamos, New Mexico 87545
Contract:	W-7405-ENG-36
Title:	IV. Space Plasma Physics
Person in Charge:	D. N. Baker

Scope of Work

The objective of this program is to analyze and interpret existing satellite data from the solar wind and earth's magnetosphere to yield an understanding of physical mechanisms and long-term effects of sun-earth coupling through the solar wind and to understand sources of free energy in these plasma particle velocity distributions. Since the solar wind and magnetospheric plasmas are the media through which solar-generated disturbances propagate and in which solar wind convection energy is stored and subsequently released to the auroral ionospheres, these studies help us understand the coupling of solar variations to the near-earth environment. This research relates to the Department of Energy's missions through applications to plasma physics and magnetohydrodynamics (MHD) problems relevant to fusion energy technology, understanding long-term solar wind and earth climate variability, and future space-based energy technologies.

A. Energy Transport in Space Plasma (S. P. Gary and W. C. Feldman)

The long-term goals of this research are to describe the structure of and flow of plasma energy in the solar wind and the earth's bow shock, magnetosphere, and ionosphere. Specific aims include determining the properties of the electron and ion distribution functions in the solar wind in order to better understand heating and transport processes, and understanding solar wind-magnetosphere coupling through fundamental studies of plasma instabilities and transport in and near the earth's bow shock, magnetosphere, and ionosphere.

Our most important research of 1983 has been a comprehensive survey of electromagnetic ion beam instabilities near collisionless shocks such as the earth's bow shock and interplanetary shocks. Our work has shown there are four different kinds of beam driven instabilities, and has demonstrated the parameter regimes in which each is important. These results have important implications for understanding how collisionless shocks accelerate ions to high energies, and may bear on the important astrophysical question of cosmic ray acceleration by interstellar shock generated by supernovae.

B. Electrodynamical Aspects of the Solar Wind-Magnetosphere Integration (E. W. Hones, Jr.)

The interaction of the solar wind with the earth's magnetosphere is in the nature of an electrical generator, i.e., a conducting medium (in this case the solar wind plasma) moves through a magnetic field (in this case the earth's magnetic field), giving up its momentum in the generation of electrical currents. The solar wind-magnetosphere system is much like an MHD generator of unusual geometrical design. But it has the additional feature that it can store the electrical energy that it creates in the form of magnetic fields and this it does in the geomagnetic tail. Unlimited energy cannot be stored in the tail and excess energy is released intermittently in spasmodic fashion which part of the tail plasma sheet is severed from earth by magnetic reconnection. This process occurs during (and is the cause of) a magnetospheric substorm in which some energy is deposited in the polar ionosphere and a comparable or greater amount is returned to the solar wind as the severed plasma sheet in the form of a plasmoid (a plasma structure threaded with closed magnetic loops) flows downstream out of the tail.

There are two major results of our work during this year: 1) Working with data from the ISEE-3 satellite for (~ 1.5 million kilometers) down the tail we identified the substorm-generated plasmoids passing that distant location; and 2) We held a Chapman Conference on Magnetic Reconnection at the Los Alamos National Laboratory. The Conference was hailed as an outstanding success and most of the papers will be published in an American Geophysical Union Geophysical Monograph entitled Magnetic Reconnection in Space and Laboratory Plasmas. The book will be available in May 1984.

C. Theory of Energetic Acceleration and Precipitation from the Terrestrial Magnetosphere (D. N. Baker and M. F. Thomsen)

In this research effort we address the details of fundamental acceleration processes and resonant wave-particle interactions in the earth's outer radiation zone. These aspects of energetic particle studies deal specifically with the problem of how energetic electrons are generated and subsequently lost from the magnetosphere into the auroral ionosphere.

During this year we re-examined recent theories which ascribe banded chorus emissions to whistler instabilities driven by the presence of an energetic electron loss cone feature. We have improved this theory by using realistic observed distribution functions and by solving the dispersion relation exactly for the case of parallel propagation. We have also used concurrent data from the Los Alamos geostationary orbit energetic electron particle sensors and ISEE-1 instruments to determine those cases where high fluxes of trapped electrons were present and ISEE was within ±1 hour of local time of a synchronous orbit spacecraft. Several candidate events have been identified and analyzed.

We have further extended our understanding of solar wind-magnetosphere interactions through the use of statistical studies. In one class of investigations using the method of linear prediction filtering, we found that the magnetosphere responds to solar wind changes on two characteristic time scales: 20 minutes and 60 minutes. The 20 minute scale represents direct driving of magnetospheric currents by the solar wind while the 60 minute response is due to storage of energy in the magnetotail (for ~ 1 hour) followed by a sudden release of this energy through substorm reconnection.

Much of the work during the past year has been directed toward a determination of where, when, and how magnetospheric reconnection occurs and how energetic particles are accelerated in this process. In one such study we have examined very detailed plasma, energetic particle, and magnetic field reconnection signatures at ~ 30 R_E geocentric distance in the plasma sheet. We find good direct evidence of strong electron acceleration and heating in many of our reconnection events. In other studies we have used plasma composition and energetic particle drifts in the earth's magnetic field to identify the location and spatial extent of substorm reconnection. We have also used these results to determine whether the plasma in the outer magnetosphere during each event originated in the solar wind or the ionosphere. Our geostationary orbit particles are accelerated and shy plasma sheet instabilities develop in certain regions.

All of these sorts of substorm-related topics have been reviewed by us in a major solar-terrestrial physics document called Solar Terrestrial Physics - Present and Future to be published by NASA. Our contribution on substorms constitutes one of the chapters of this book and summarizes the present understanding of substorm processes.

Contractor: OAK RIDGE NATIONAL LABORATORY
Union Carbide Corporation
Oak Ridge, Tennessee 37830

Contract: W-7405-eng-26

Title: Geochemistry of Crustal Processes to High Temperatures and Pressures

Person in Charge: Robert E. Mesmer

Scope of Work

The major goal of the program is to better understand the chemical and physical processes operating in the aqueous and molten silicate fluids that are responsible for the distributions of elements in the earth's crust. Our principal avenue to this goal is experimental studies of selected natural and analogue chemical systems at temperature and pressure conditions simulating crustal environments to depths of 18 km.

Experiments are conducted on the phase equilibria, crystallization kinetics, and elemental/isotopic partitioning of rock-forming silicate systems over temperatures ranging from 500 to 1400°C and pressures to 500 MPa under controlled redox conditions to develop understanding of magmatic/hydrothermal processes. Homogeneous and heterogeneous hydrothermal experimental studies of major and minor crustal components are used to derive the thermodynamic and kinetic data required to develop models for the distribution and mobilities of elements in the upper few kilometers of the crust. This research provides insight into problems associated with energy transfer in magmatic/hydrothermal systems, volcanic processes, mineral resource exploration, enhanced techniques for oil and ore recovery, nuclear waste isolation, geothermal energy and development of ceramic structural materials.

A. Silicate Melt Geochemistry (Naney)

Iron Redox Equilibration Kinetics in Silicate Liquids (with S. E. Swanson, University of Alaska).

A series of experiments with three silicate liquids derived by melting natural volcanic rocks (basalt, andesite, and rhyolite) were conducted at 0.1 MPa (1 atm), 1243°C and two oxygen fugacities: log f_{O_2} = -6.08 and -7.83 (QFM) in a CO/CO_2 gas-mixing vertical tube furnace. Minimum equilibration times are 500 and 1000 min for the basalt and andesite respectively. Equilibrium times reported here are comparable to durations cited in the literature for experiments with basalt and andesite.

Ferrous/ferric ratios in samples of rhyolite showed no indication of reaching equilibrium with furnace oxygen fugacity in experiments of up to 5900 min duration. Experiments with crushed rhyolite showed oxidation of the melt related to the interaction of liquid formed during heating with air trapped between the grains of the original sample pellet. This phenomenon was also observed in the andesite and basalt experiments. However, unlike the basalt and andesite melts, the ferrous/ferric ratios of rhyolites showed no further changes following initial oxidation. Iron redox behavior in natural rhyolites is similar to that observed in experiments with rhyolites. Oxidation of rhyolite ash-flows is probably related to high temperature air-ash reaction during or immediately following eruption. In contrast, massive glassy rhyolites (flows and domes) show little variation in bulk ferrous/ferric ratio--despite the fact that constituent Fe-Ti oxides may show a wide range of compositions--which suggests that these massive rhyolites are insensitive to external changes in oxygen fugacity.

Stability of "Magmatic" Epidote in Granitic Rock Systems. The stability of epidote $[Ca_2Al_2FeSi_3O_{12}(OH)]$ is being investigated in synthetic analogs of natural granite and granodiorite compositions. Experiments are currently being conducted between 400°C and 600°C, over the pressure range 200-400 MPa to define the stability limits of epidote under subsolidus conditions. The hydrogoen-service internally heated pressure vessel, which permits control of redox conditions over a wide range of f_{O_2}-T conditions, is being used for this study. Results of recent experiments indicate that epidote is stable to at least 500°C and 400 MPa at relatively oxidizing conditions (Ni-NiO $< f_{O_2} <$ Mt-Hm) in the composition investigated. However, under more reducing conditions ($f_{O_2} <$ Ni-NiO) epidote is unstable at 550°C and 400 MPa. These experiments are doped with uranium to permit simultaneous investigation of the chemical partitioning of this actinide.

Geochemistry of Silicic Magma Systems (with W. C. Luth and J. C. Eichelberger, Sandia National Laboratories). A suite of hydrous rhyolitic glasses from tephra depostis of Little Glass Mtn., California, were analyzed at ORNL for ferrous and ferric iron using a colorimetric method adapted to analyze micro-sample (10-30 mg). These samples which contained H_2O contents ranging from 0.15 to 1.79 wt. pct. showed no significant variation in ferrous and ferric iron contents. This is an interesting finding in light of the commonly held opinion that hydrous volcanic glasses tend to be more oxidized than anhydrous glasses.

B. Hydrothermal Geochemistry - Homogeneous Equilibria (Wesolowski, Drummond)

Second Dissociation Constant of Sulfuric Acid in 1.0 m NaCl from 75-295°C. These experiments were performed in a hydrogen electrode emf cell and they demonstrate that sulfate species will persist metastably in a hydrogen atmosphere long enough to make precise measurements of the sulfate/bisulfate equilibria to 300°C. The present results represent the only direct measurements of sulfate hydrolysis in chloride media at elevated temperatures and are the first of a series of such experiments that will extend over a wide range of salinity (0.1 to 5 m) and include NaCl-MgCl$_2$ mixtures.

Above 200°C the equilibrium quotients of Marshall for the reaction HSO_4^- SO_4^{2-} + H^+ in Ca^{2+}-H^+-HSO_4^--SO_4^{2-} media match those in NaCl media. These two data sets differ by as much as 50% at lower temperatures suggesting important media effects.

C. Hydrothermal Geochemistry - Heterogeneous Equilibria (Drummond, Dickson)

Hydrolysis of Magnesium and Brucite Solubility in Aqueous Sodium Chloride Solutions at Elevated Temperatures by EMP (with P. Brown, Western Australia University). A series of potentiometric titrations in the hydrogen electrode emf cell have been carried out to measure the solubility of brucite ($MG(OH)_2$) and the hydrolysis of Mg^{2+} in aqueous sodium chloride solutions from 60 to 200°C. Most of the titration data were taken subsequent to brucite precipitation. These data were analyzed by least squares regression in terms of the solubility product of brucite and many of the possible $Mg_x(OH)_y$ hydrolysis products. Separate solubility experiments in strong base (at both 60° and 200°C) gave no indication of amphoteric solubility and hence negate the possibility of the formation of even minute quantities of negatively charged $Mg_x(OH)_y$ species in the titration experiments. Consequently, the titration data are described solely in terms of the solubility product of brucite. For the entire data set of solubility quotients 3 was about 0.05 log units. The enthalpy for the reaction $MG(OH)_2(s) + 2H^+$ $Mg^{2+} + 2H_2O$ in both 0.1 and 1.0 m NaCl media is 26.2 kcal/mole which agrees favorably with the estimate of 27.3 by Baes and Mesmer (1981).

Thermal Decarboxylation of Acetate: Boundary Conditions for the Role of Acetate in the Primary Migration of Natural Gas. In and effort to understand the kinetics of the thermal decarboxylation of acetate and the role of catalysis, a series of laboratory experiments were conducted to measure the rate constant for the decomposition of acetic acid in the presence of a variety of materials including gold, titanium, stainless steel, silica, montmorillonite and magnetite. Activation energies for decarboxylation range from about 8 kcal/mole in stainless steel to 57 kcal/mole in treated titanium vessels. Extrapolated rate constants at 100°C differ by more than thirteen orders of magnitude between the stainless steel and the least catalyzed titanium experiments. Methane and carbon dioxide were the predominant reaction products of these experiments but mass spectrometric analysis revealed concentrations of carbon monoxide, hydrogen, and hydrocarbons (apparent masses range from 29 to 56) amounting to as much as 40 mole percent of the total volatile products, depending on the catalyst. Gold, titanium, and pure montmorillonite were the least active catalysts while stainless steel, silica, and magnetite showed marked catalytic effects. The reactions were first order in acetate except for the experiments with silica and magnetite which were zero order. With this recent advance in the understanding of the chemical kinetics of acetate decarboxylation, it is possible to assess the role of acetate in the primary migration of natural gas. The appropriate physical, chemical, and geological constraints on this process were considered and integrated via a computer model that couples basin subsidence, compaction and fluid flow parameters with the chemical constraints dictated by the experimental kinetic data. This analysis shows that acetate can account for substantial gas migration from source rocks in the early catagenic stages of kerogen degradation at depths around 3 km and temperatures of 110 + 20°C.

Quartz Solution/Dissolution. The reaction of quartz grains with H_2O and NaCl were studied at 200, 220, and 250°C, 20 MPa and over times ranging from 20 to 200 hrs (av. 144 hrs). Some experimental difficulties that were encountered early in the year were worked out. A total of 15 experiments were done which involved 182 samplings and analyses for SiO_2. Experiments used double titanium alloy reaction vessels held in one furnace that were connected to permit transfer of fluid from the top of one vessel (reservoir vessel) to the bottom of the other (reaction vessel) during sampling. Experiments were done at several mass-ratios of quartz to solution: 5.0, 1.2 and 0.22 in g·Qtz per g·H_2O. Two grain size ranges (+80 and 35-80 mesh) and 3 total surface areas of the quartz were used (0.415, 0.177, and 0.0445 M^2). Part of the experiments with quartz-filled vessels were static; all other were rocked through vertical several times per minute. The experimental data have been processed to determine equilibrium solubilities and kinetic reaction steps and rates. Rates of reactions of initially undersaturated solution with quartz are rapid compared to reactions of supersaturated solutions. The behavior of quartz-solution systems reflects the prior events (sequences of variations in time, temperature, pressure, and concentrations). Apparently a new solid phase, probably metastable, forms as layers of the quartz, as has been reported also by other workers. The surface coatings evidently are pervasive and tenacious. They prevent quartz surfaces form interacting directly with solution so long as they are present. Apparent orders calculated for quartz reactions range from 1.00 to 1.50 for undersaturated solution and to 10 and above for supersaturated ones.

D. Hydrothermal Geochemistry - Modeling (Cole, Wesolowski, Drummond)

Geochemistry of Tungsten in Hydrothermal fluids Experimental studies of the hydrolysis of tungsten (VI) in NaCl solutions to 300°C conducted at this laboratory have enabled us to develop a quantitative model for the transport and deposition of scheelite ($CaWO_4$) in ore and geothermal systems as a function of temperature, pressure, ionic strength and acidity. The model has been demonstrated to adequately explain the occurrence of ore grade levels of this important strategic and industrial commodity in several types of ore systems ranging from 0.1 to >10 MPa and 100 to 500°C. The important variables controlling solubility have been identified as temperature and ionic strength in low P-T regimes and proton concentration at higher pressures and temperatures. However, the interplay of these variables is complex and the physicochemical conditions of the depositional system must be well characterized.

Modeling Activity Coefficients in Hydrothermal Solutions. Recently, largely through the efforts of researchers at ORNL, a fairly complete body of stoichiometric activity coefficient data has become available for the major components of natural hydrothermal solutions in NaCl media to 300°C. It is clear from these data that, up to 300°C, the salts in natural hydrothermal solutions behave as if they are predominantly ionized and that NaCl is a good model substance for the activity coefficients of these components. As a consequence, it has been possible to systematize these data via a computer program that, in contrast to the ion-pair approach used historically by most geochemists, allows the activity coefficients of these components to be computed accurately, unambiguously and simply.

Oxygen Isotopic Exchange Accompanying Surface Reactions and Diffusion (in collaboration with H. Ohmoto and A. C. Lasaga, Penn State University).

Oxygen isotopic exchange between minerals and fluids proceeds through two mechanisms: (1) surface reactions (dissolution, precipitation) and (2) diffusion of oxygen-bearing species along lattice planes or crystal imperfections. The rate constants for the first type of mechanism are related as follows: $r = -\ln (1-F)(WS)/(W + S)(A)(t)$ where W and S are the moles of oxygen in the solution and mineral, respectively, A is the surface area of the mineral (m^2), t is time (sec) and F is the fraction of isotopic exchange. Examination of the published experimental data on oxygen isotopic exchange reactions between various phases (e.g., silicates, carbonates, sulfates) and aqueous fluids using the above equation yields rate constants of between 10^{-4} and 10^{-8} moles m^{-2} sec^{-1} in the temperature range of 800 to 250°C, and activation energies of between 8 and 22 kcal mol^{-1}. Rates of oxygen isotopic exchange accompanying diffusion of oxygen-bearing compounds through mineral lattices are also calculated from published experimental data using equations that take into account fluid/mineral mass ratios of the systems. These data suggest that oxygen isotopic exchange reactions between fluids and rocks in natural systems may proceed in two steps: the first through a surface-controlled mechanism when the fluids and minerals are out of chemical equilibrium, and then through a diffusional mechanism once the systems attain chemical equilibrium.

Partitioning of Hydrogen and Oxygen Isotopes between Aqueous Electrolytes and Coexisting Vapor. The existing experimental data on the fractionation of oxygen and hydrogen isotopes between liquid and vapor in pure fluids and in electrolyte solutions have been critically reviewed. D/H and $^{18}O/^{16}O$ fractionations between pure liquid and vapor at near infinite dilution in $H_2{}^{16}O$ from 0-200°C can be accurately modeled by the measured vapor pressure ratios of the isotopic liquids $D_2{}^{16}O$ and $H_2{}^{18}O$ relative to pure $H_2{}^{16}O$, assuming ideal mixing in both phases and accounting for the disproportionation reaction $H_2{}^{16}O + D_2{}^{16}O \quad 2HD^{16}O$. Above 150°C, the calculated fractionations for D/H partitioning are significantly improved by correcting the vapor pressures for gas of liquid D_2O in liquid H_2O. At temperatures above 300°C, additional corrections are necessary for nonideal mixing and molar volume effects. At geothermal temperatures (- 100-300°C) large liquid-vapor isotope fractionations occur, and thus phase separation (i.e., boiling, condensation) must be considered in quantitative modeling of fluid-rock isotopic exchange in dynamic systems. Data on fractionation of oxygen and hydrogen between vapor and high salinity brines at elevated temperatures are sparse and conflicting. This information is necessary for the interpretation of geochemical processes based on isotope measurements.

Contractor: PACIFIC NORTHWEST LABORATORY
Battelle Memorial Institute
Richland, Washington 99352

Contract: DE-AC06-76RLO 1830

Title: I. Remote Sensing: Geoscience Data Analysis and Integration

Persons in Charge: G. E. Wukelic and H. P. Foote

Scope of Work

Since 1976, PNL has been conducting research in areas of remote sensing, image processing, and computer graphics most relevant to the geoscientific interests of the Department of Energy. The goal of this task is to develop practical interactive computer techniques for processing and analyzing combinations of remote sensing and geoscience data so scientisits can interpret more complex data combinations more completely and more rapidly. Successful techniques are being integrated into basic research and technology programs involving resource discovery, national security, energy development and utilization, conservation of the environment, and the safety objectives of the Department of Energy.

The current scope of research responsibilities involves:

(A) Maintaining cognizance and acquiring appropriate remote sensing and geoscience data sets to support continuing research efforts;

(B) Upgrading computer capabilities (hardware and software), as required, to advance the state of the art in digital processing, analysis, and display of remote sensing (imagery) and geoscience (point, line, and map) data;

(C) Demonstrating and integrating experimentally developed techniques within basic research and technology programs internal and external to DOE.

A. Remote Sensing and Geoscience Data Base Expansion

(H. P. Foote, S. C. Blair, and G. E. Wukelic)

Several new data sets have recently been acquired and processed. Remote sensing examples include day and night Landsat seven-band thematic mapper (TM) scenes, Heat Capacity Mapper Mission (HCMM) data, and Thermal Infrared Mapping Spectrometer (TIMS) data from selected areas of DOE research and development interests. Current emphasis is on acquiring and experimenting with the shuttle imaging radar (SIR) and the

French (high-resolution stereo) SPOT data to be acquired in the fall of 1984.

Additional geologic and geophysical data items and maps to support primarily the preparation of more advanced CSDP demonstration products were acquired and selectively digitized. Digital ocean bottom topography (bathymetric) and ocean surface (radar altimetry) data for the coastal region of Washington State have been acquired to test ocean data analysis software programs under development.

B. Image Processing/Computer Graphics Software Developments

(H. P. Foote, S. C. Blair, and G. M. Petrie)

1. Image Enhancement, Data Integration/Analysis and Classification Programs. New and/or improved programs (e.g., Principal Component, Intensity-Hue-Saturation, etc.) have been added to upgrade the system's image enhancement, spectral classification, and change detection functions for general usage. Current emphasis is on upgrading interactive analysis programs to maximize the usefulness of the Landsat seven-band thematic mapper data capability for energy related applications, both qualitatively and quantitatively.

2. Transition to VAX 11/780 Operations. We are currently involved in transferring computationally intensive programs to the VAX 11/780 - array processor combination and incorporating additional NASA image-processing software developed at Goddard specifically for manipulating Landsat thematic mapper data.

3. Computer-Generated Shaded Relief Maps. During 1983, a software program was developed and tested for generating gray-scale and color-coded relief maps for both large and site-specific areas using various resolution levels of available terrain data. The program is capable of generating a variety of shading options simply by altering the solar illumination angle and of emphasizing area of lower topographic relief; both of which have potential for inexpensively enhancing surface features of geologic interest not normally seen in standard satellite images. This program was used to prepare a series of shaded relief maps for the 1983 CSDP Long Valley, CA Workshop.

4. Oblique-Multiparameter Stereo Graphics. A computer program has been successfully developed for improving 3-D integrated (remote sensing and geoscience) data displays by incorporating the capability to generate a variety of viewing perspectives other than vertical. This results in multiparameter stereo graphics, which more closely resemble on-the-surface viewing and this should improve the interpretation value of such

products. This program was also used to prepare a series of combined Landsat, topography, and geology stereo graphics for the 1983 CSDP Long Valley, CA Workshop.

C. Demonstration and Application of Task-Developed Capabilities (H. P. Foote, G. E. Wukelic, S. C. Blair, and G. M. Petrie)

1. Evaluation of Landsat Thematic Mapper Geoscience Data-Use Implications. Initial processing, analysis, and evaluation of Landsat TM data started in FY83 as part of a cooperative PNL-NASA GSFC agreement and will continue until April 1983 with the successful launch of Landsat-5 on March 1, 1984. Efforts to date have emphasized the qualitative potentialities of single band, multiband (composited), and ratioed TM products. Published results to date have emphasized the qualitative potentialities of single band, multiband (composited), and ratioed TM products. Published results to date have demonstrated and documented the utility of the increased spectral and spatial capabilities of the thematic mapper for siting and monitoring major energy facilites. Future research will stress the quantitative uses of TM radiometric data and associated error factors (e.g., data processing, atmospheric, and sub-pixel effects) and how they can be modeled to improve TM use for surface-temperature determinations.

2. Application to Midscale Geologic Features. The use of PNL computer image processing and manipulation techniques for analyzing rock features are being examined. Thirteen rock samples were sectioned, photographed, and digitized into 512 x 512 picture elements (pixels). Existing image processing programs were then used to classify each pixel as either grain or pore space. Further software development allowed the number of distinct grains (or pores) contained in each image to be determined and to associate each pixel with the parent grain (or pore) space. Each pore could then be characterized by its area, shape, and direction. Plans include extending this 2-D test to a 3-D representation of the rock structure.

3. Application to Geoscience Studies in the State of Washington. We have recently completed a digital, high-resolution topography mosaic for the state of Washington to use in preparing a series of integrated geoscience data products. In this demonstration, 36 one-degree-square DMA digital elevation files were resampled to form one file in a Lambert conic projection. The file covers the region from longitude 125°W to 116°W and latitude 45°N to 49°N. The grid spacing for the file is 154 m, resulting in array dimensions of 4608 by 3000 pixels. Thus, the file contains about 13.8 million elevation values. The ground resolution of the file is approximately

five times greater than any other single elevation file for the State. The new elevation file will find application in several geologic and geophysical studies within the State. Shaded relief maps can be computed from the elevation data from any desired illumination angle. We are in contact with the geology department at Washington State University, where somewhat similar work is being done with physical relief models. We will prepare digital relief maps from several lighting directions for comparison with the physical models.

4. Application to CSDP. The CSDP represents an ideal opportunity to obtain expert opinions as to the geoscientific interpretation significance of the experimental geodata analyses and display techniques being developed and tested under this task. Accordingly, an initial series of geodata demonstration products were prepared in support of the Valles Caldera Workshop (1982) and the Mono Craters-Long Valley Workshop (1983). These products were well received by the participants, and we are currently emphasizing 1) the acquisition of Landsat thematic mapper data for these and other CSDP sites (under the NASA-PNL LIDQA Program Agreement) and 2) the interaction with CSDP participants to acquire more geoscientific data for preparation of more extensive data integration products in the near future.

Contractor:	PACIFIC NORTHWEST LABORATORY Battelle Memorial Institute Richland, Washington 99352
Contract:	DE-AC06-76RLO 1830
Title:	II. DOE Insolation/Aeronomy Studies
Person in Charge:	G. M. Stokes and E. W. Kleckner

Scope of Work

The current program concentrates on the areas of aeronomy in the upper atmosphere and on insolation and radiative properties of the lower atmosphere. In particular, the aeronomy program is concerned with energy transport and interactions within the complex interface between the plasmasphere/magnetosphere regions and the ionosphere/upper atmosphere regions. Significant advances have been achieved over the past two decades in expanding our basic knowledge of the earth's atmosphere and magnetosphere and the sun as an interacting system. It is important that the physics of this coupling region be well understood in order to obtain definitive solar-terrestrial cause-effect relationships.

The insolation program relies on a data base of direct and diffuse solar radiation measurements made in visible and near-infrared spectral passbands. The research focuses on two goals. One is to quantify the spectral characteristics of scattered and direct sunlight. This is germane to energy generation solar technologies such as daylighting. The primary emphasis of the insolation task is on the characterization of the influence of trace species in the troposphere and lower stratosphere on solar radiation. These man-made or naturally produced trace species include aerosols, molecules, and clouds.

A. Insolation Studies

(J. J. Michalsky, N. R. Larson, and E. W. Kleckner)

Significant progress was made in the characterization of the continuous solar spectrum from discrete sampling of that spectrum. One goal of the insolation work is to develop low-cost instrumentation and data reduction techniques which can be used to provide adequate spectral information for technologies which are sensitive to a broad, continuous spectrum. These include materials research, biomass, daylighting, and photovoltaics among others. Two mathematical methods for using discrete filter measurements to generate continuous spectra are described in a paper accepted for publication in Solar Energy. The effectiveness of the procedures are demonstrated to some degree by using the technique on simulated filter measurements. A second paper has been drafted which extends the validation effort by comparing modeled spectra using measured or estimated aerosol, water vapor, and ozone data. The estimated spectrum based on filter measurements is also compared to simultaneous spectroradiometric measurements in that paper. The agreement is within the error bounds for the spectroradiometric measurements and for the modeled spectra.

The major activity in the insolation work this past year had been on volcanically produced aerosols. A data base which extends to the Spring of 1978 at PNL has been used to establish a non-volcanically perturbed background aerosol data base. From these measurements it has been found that monthly-averaged aerosol optical depths are reproducible from year-to-year when there is no volcanic perturbation of the aerosol burden of the troposphere or stratosphere. These background measurements helped establish the non-significance of the climatic impact of the Mount St. Helens eruptions in earlier work. The past two years it has been used to monitor the evolution during the Spring of 1982. The first year's data (following El Chichon's eruption) which consist of differences between pre- and post-eruption optical depths as a function of wavelength have been inverted for size distribution in a collaboration with University of Arizona scientists. A publication on these results appeared in the January issue of Geophysical Research Letters. We are about to complete the reduction of a second year's data set. The influence of the El Chichon cloud is quite easy to discern through 1983. The interest of this volcano is not only the attenuation of sunlight by the cloud, but more importantly, the inferred sizes of the stratospheric aerosols. In the first year they evolved to sizes that were much larger than modeled volcanic size distributions. These larger sizes may affect the surface temperature in an unexpected manner. This unexpected behavior in size evolution should warn us about how we regard historical volcanoes and our models of those eruptions' influence on climate.

B. Aeronomy Studies (E. W. Kleckner, D. W. Slater, N. R. Larson)

Solar-terrestrial interactions shape and link the three major regions of near earth space: the magnetosphere, the ionosphere, and the atmosphere. A major goal of the aeronomy program is to investigate the coupling of the ionosphere, plasmasphere, and magnetosphere. To accomplish this, a network of computer-controlled, automated photometers has been maintained to acquire synoptic observations of the aurora and airglow. These, in turn, provide valuable information concerning the complex question of energy transport within this system, and the system's response to ever changing conditions.

One type of phenomenon, Stable Auroral Red (SAR) arcs, has been the subject of extensive investigation during the past year. These midlatitude features constitute the ionospheric response to energy influx from the equatorial plasmapause region. Such energy input distributed on a global scale can be expected to have significant effects within the ionosphere, effects which are currently being investigated. Work in this area has proceeded from analysis started last year which suggested an association of SAR arcs with precipitating suprathermal (< 10ev) electrons as detected by the Dynamics Explorer -1 and -2 spacecraft. In cooperation with Southwest Research Institute, we have identified a one-to-one correspondence of these precipitating electrons and SAR arcs for approximately 30 individual events. As shown by earlier analysis, heating of the ionosphere/thermosphere within SAR arcs by this energy influx can lead to a "fountain effect," i.e., a thermally driven convection cell capable of injecting enhanced densities of N_2 from low altitudes into regions within the above SAR arcs. We have initiated study of satellite measurements of atmospheric neutral species within these locations for comparison with empirically derived atmospheric models. Initial results indicate significant compositional perturbations due to these localized heat sinks.

The comprehensive catalog of SAR arc events as detected by the PNL photometer network has been made available to researchers as a PNL report.

Final construction, software development, and testing of a multichannel, meridian scanning photometer is nearing completion. The instrument is capable of parallel processing four independent photometric channels at the high speed needed for time-resolved of the aurorae and airglow. The parallel acquisition feature will allow direct use of intensity ratios in the determination of the energy spectrum of precipitating particles. An additional system, centered around a high resolution spectrometer, is also being brought on line. This will allow observation of OH temperatures and densities. In particular, we are focusing on measurements of processes in the 80-95 km region near the mesopause.

Data processing is current with all units, and archival quality magnetic tapes containing the data are routinely prepared. Access by researchers to this data base has been facilitated by the introduction of an easy-to-use retrieval system.

Contractor:	PACIFIC NORTWEST LABORATORIES Battelle Memorial Institute Richland, Washington 99352
Contract:	DE-AC06-76RLO 1830
Title:	III. Chemical Migration by Contact Metamorphism in Granite - Country Rocks
Person in Charge:	J. C. Laul

Scope of Work

The main objective is to investigate the relative migration and transport mechanism of major, minor, and particularly trace elements during contact metamorphism between granite pegmatites and surrounding country rocks. Specific emphasis will be on the rare earth elements (REE) -- Ba, Sr, K, As, Sb, Pb, Cl, Rb, Cs, Zr, Hf, Ni, Th, and U. The applications of this study may enable us to understand and predict the long-term (10^3 to 10^7 years) behavior and movement of radionuclide in diverse geologically confined nuclear waste.

The first geological site was the granite intrusion at Notch Peak in Southwest Utah. Some of the important findings were: 1) the granite stock is composed of three concentric sequentially intruded rock types, 2) maximum temperature near the contact between the quartz monzonite intrusion and the Cambrian sediments was 575-600°C, 3) relative to silts, limestones were impermeable to fluids and the flow of fluids was confined to silt beds and fractures, and 4) in silt, elements Na, K, Rb, Ba, Sr, As, Sb, Pb, and Cs have migrated over tens of meters, while there is no detectable migration of REE, V, Cr, Sc, Zr, Hf, and Al.

The second geological site is pegmatite - country rocks in the Black Hills, South Dakota. Five different pegmatites have been chosen to address (a) composition of fluids, (b) capability of dispensing fluids into country rocks, and (c) partitioning of mobile elements between mineral phases and fluids derived from pegmatites. Preliminary studies of the Tin Mountain, Etta, and Bob Ingersoll pegmatites show that there is virtually no migration of REE, Al, V, Sc, Cr, Hf, and Th elements. On the other hand, elements K, Li, Rb, Cs, As, Sb, Zn, and Pb have migrated 4 to 90 meters. The degree of migration varies depending on the element. Minerals biotite and muscovite are effective trace element traps for Li, Rb, and Cs. However, biotite has a greater affinity for Li, Rb, and Cs than muscovite and their relative affinities can be explained in terms of crystal chemistry. The REE concentrations in biotite and muscovite are high and indigenous. Similar types of chemical studies in other pegmatites emphasizing minerals such as apatite and tourmaline as a recorder of melt/fluid evolution are under progress. The chemical data on some 40 major and minor trace elements are obtained by neutron activation analysis and x-ray fluorescence.

This study is in collaboration with J. J. Papike of South Dakota School of Mines and Technology, Rapid City, South Dakota, who will obtain mineralogic and petrologic data on the same samples.

Contractor:	SANDIA NATIONAL LABORATORIES Albuquerque, New Mexico 87185
Contract:	DE-AC04-76DP00789
Title:	I. Continental Scientific Drilling Program Thermal Regimes
Person in Charge:	W. C. Luth

Scope of Work

Research conducted under the auspices of the Continental Scientific Drilling Program (CSDP) - Thermal Regimes sub-program at Sandia involves both generic and site specific activities as well as technology development and operation of a Thermal Regimes Research Drilling Office. Generic supportive research efforts include: development and testing of advanced thermal geophysical techniques; analysis of surface manifestation of subsurface magmatic emplacement; and a portion of the research conducted under III (Geochemistry Research) bearing on energy and mass transfer within, and between, hydrothermal and magma systems. Site specific research is concentrated at the Mono Craters-Long Valley, California, site and involves a number of non-Sandia participants. Recognition of the need for advanced technology to obtain scientific data in the hostile hydrothermal-magma transition zone resulted in a research program in drilling, logging, and instrumentation to provide the base for technology development. A Research Drilling Office has been established to implement the drilling activities of the CSDP-Thermal Regimes sub-program. The first major activity of the Research Drilling Office will be to provide support for the joint laboratory (SNL, LANL, LBL, LLNL) shallow drilling program.

A. CSDP - Thermal Geophysical Techniques (J. C. Dunn and H. C. Hardee)

The objective of this research is to develop and refine thermal geophysical techniques in order to characterize and understand in situ thermal processes near high temperature heat sources in the crust. Such thermal geophysical techniques include measurement and analysis of thermal and fluid transport in regions where natural convection heat transfer and/or ground water flow in aquifers significantly alter subsurface temperature profiles. Current research is presently concentrated in two areas:

(1) A convective heat flow sensor is being developed for use in permeable subsurface zones. A prototype downhole instrument was used to measure ground water velocities and convective heat flow in Long Valley, California. An improved downhole instrument has been calibrated in a permeable test bed at velocities as low as 10^{-7} m/s. Several small scale versions

of the instrument have been constructed to test improved methods of velocity measurement in a permeable medium.

(2) Thermopile heat flux sensors are being used in regions where surficial heat flow is relatively high. In such regions, normal surface temperature variation effects become unimportant at very shallow depths. The sensors can, therefore, be emplaced by simple digging as opposed to the normal requirement of drilling heat flow holes. In addition to speed of measurement, the thermopile method of heat flow measurement gives a direct measurement of vertical heat flow essentially at a point. This eliminates the need to obtain gradients from temperature measurements over a finite vertical extent. The sensors have been used to obtain heat flow profiles over a suspected intrusion in the East Rift Zone of Kilauea volcano, Hawaii. Here 20 heat flow measurements were taken with 4 thermopile sensors in a time period of two days.

B. Magmatic Emplacement (C. R. Carrigan)

The characterization of the geology and physics of a geothermal system requires treating the problem of both the thermal and dynamical evolution of magmatic reservoirs. How such reservoirs evolve is dependent in part upon heat transfer processes in the country rock exterior to a magma body. A model for estimating heat transfer and infiltration within a two-phase (liquid/vapor) hydrothermal zone adjacent to a dike has recently been developed using an engineering type heat transfer analysis. The model is best applied to shallow geothermal zones which are most accessible to drilling and which are of interest from a hazards perspective. The model predicts maximum dike solidification rates of about 1 meter/yr for reasonable permeabilities.

The interior problem of thermal convection in a cooling reservoir is being studied using both finite element and parameterized schemes. For 100 M rhyolite sills, the more approximate parameterized models are found to be in reasonable agreement with the more rigorous 2-D finite element models. The parameterized models can in principle be extended to model the thermal regimes of cooling magma bodies which are beyond the parameter ranges treated by finite element or difference formulations. In terms of computer resources, they are also much less costly to produce.

C. CSDP Mono Craters-Long Valley (CA) Site Assessment (J. C. Eichelberger and J. B. Rundle)

With its long history of active volcanism, and its current tectonism and seismicity, the Mono Craters-Long Valley region is important as a potential site for deep continental drilling. For the past two years, assessment of this site as a crustal thermal regimes target for drilling has been conducted using a variety of geophysical, geochemical and petrologic techniques. Investigations under this program are being conducted by a variety of National Laboratories, the U.S. Geological Survey, Academic Institutions, and private industry.

Specific investigations include a high resolution seismic refraction profile covering the entire Long Valley caldera and the Mono Craters-Inyo Domes chain of recent extrusions; establishment and reobservation of a dense network of high precision gravity benchmarks throughout the entire Long Valley-Mono Craters area; passive seismicity recording; temperature and heat flow observations; and geochemical and isotopic analyses of carefully sampled young ($< 10^3$ yr) volcanic glasses. Data examined and analyzed to date indicate the probable existence of shallow magma within the caldera, and that surface samples show a pattern of degassing of volatiles indicative of the physics of emplacement of the recent extrusives.

D. CSDP - Drilling, Logging, and Instrumentation (H. C. Hardee and J. C. Dunn)

Drilling, logging, and instrumentation support is concerned with developing advanced logging tools and downhole instruments for CSDP and then applying these tools to answer scientific questions of interest to CSDP. Early work has concentrated on downhole seismic tools and downhole high temperature thermal probes. Shallow test holes were drilled at Long Valley for the purpose of evaluating these logging instruments.

High temperature (1200°C) thermal probes and associated cables and handling equipment are being developed for logging high temperature holes. A high temperature logging system for measuring drillhole temperatures to 800°C is in the final stages of development. This system uses a platinum RTD in a special probe assembly attached to a 2 km length of high temperature, stainless steel sheathed cable. The cable is mounted on a microprocessor controlled winch assembly and cable operation and data collection is computer controlled.

E. CSDP-Shallow Hole Investigation of Long Valley, Valles, and Salton Sea Thermal Regimes (J. C. Eichelberger)

The intrusion of magma into the upper crust, the release of heat and the development of associated hydrothermal systems are problems central to understanding the evolution of continental crust and its resources. Recent surface research into magma/hydrothermal systems under the Continental Scientific Drilling Program has concentrated on Long Valley Caldera, Valles Caldera, and the Salton Sea. All three areas contain recently active magmatic systems and currently active hydrothermal systems. A shallow drilling phase of research began at Long Valley and Valles in FY84 and will begin at Salton Sea in FY85. These holes will answer specific questions about the thermal, chemical, and mechanical behavior of magma at shallow depth, and the composition and circulation pattern of hydrothermal fluids. They will also provide a necessary step toward deeper drilling. Targets are the youngest rhyolite flow (Obsidian Dome) and its feeder conduit at Long Valley, the youngest rhyolite flow (Banco Bonito) and a hydrothermal outflow zone at Valles, and an unexplored region of the Salton Sea thermal anomaly. Laboratories participating in this program are Lawrence Berkeley, Lawrence Livermore, Los Alamos, and Sandia National Laboratories. Sandia has responsibility for drilling operations at Long Valley and the Salton Sea and for interpreting petrologic data from the Long Valley and Valles holes in terms of the degassing of rhyolitic magma. A 150 m hole was cored through Obsidian Dome and demonstrated nearly complete degassing of magma comprising the flow. Preparations are underway for the conduit hole, which will investigate vent structure and the degassing and crystallization behavior of magma emplaced under substantial (10 MPa) load. Shallow drilling at Long Valley will be succeeded by intermediate depth drilling late in FY84 under the Inyo program, which involves USGS and university participation in addition to the DOE labs.

F. Geoscience Research Drilling Office (R. K. Traeger).

The Drilling Office supports geoscientists by providing field logistics, generic hardware, drilling plan developments, and consultation for CSDP--Thermal Regimes research. In the last year, permits were obtained and contracts let to provide research holes in Long Valley, CA and the Saltôn Sea, CA. A limited instrumentation capability for borehole diagnostics is being developed and maintained. The Office is available for planning and other consultation related to drilling and instrumentation for the CSDP--Thermal Regimes.

G. Long Valley-Mono Craters (CA) Information Base (W. C. Luth and J. C. Eichelberger)

An integrated information base containing references to published geologic, geophysical, and geochemical data and interpretations is essential in considering detailed site selection for CSDP-Thermal Regimes. The information base will contain:

(1) Bibliographic information in standard reference format with keyword-based identification of data presented in the reference.

(2) A listing of researchers who are currently engaged in active research in this area, with a brief statement of type, nature, extent, and objectives of the research.

(3) Brief summary of generalized plans for future research, including shallow, intermediate and deep drilling.

The Information Base will be prepared on a stand-along microcomputer using a conventional commercial data base management system. Information will be distributed in printed form on a semi-annual basis.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Contract: DE-AC04-76DP00789

Title: II. Geophysics Research

Person in Charge: W. C. Luth

Scope of Work

Research in geophysics under this program involves modeling, experimental, and field activities leading to a more soundly based understanding of physical and mechanical processes in the earth's crust and upper mantle.

A. Crustal Strain (J. B. Rundle)

The crustal strain program has as its objective the development of methods and techniques for modeling time-dependent deformation of the earth's surface, and interpreting these data in terms of possibility of tectonic instability in a given area. Motions of a few centimeters a year, commonly observed in tectonically active areas such as the western United States, have been interpreted as due to subtle stress relaxation processes deep within the earth. These motions provide clues to the occurrence of a future event.

Computer codes have been developed which compute time-dependent surface deformation due to various sources in a layered, inelastic earth model. Additionally, other codes compute gravity, sea level, potential, and surface deformation changes due to volcanic loading of the crust; and heat flow, fluid flow and deformation due to sources of fluid pumping in a fluid-infiltrated earth model. Physics of the earthquake rupture process has also been examined using simple models of inhomogeneous faults, together with friction laws derived from laboratory failure experiments.

Gravity gradient data associated with the 1975-1977 Kilauea inflation-deflation episodes, as well as gravity change data from Long Valley have been interpreted by the use of these techniques. Work is also underway on understanding the mechanics of the earthquake cycle, both at convergent plate boundaries (subduction zones) and at transform faulted boundaries. Collaborators have included scientists at University of Tokyo, Japan, the U.S. Geological Survey, the California Institute of Technology, and the University of California, Santa Cruz.

B. Time-Dependent Deformation and Fracture of Brittle Rock (L. S. Costin and D. J. Holcomb)

This research is directed toward a basic understanding of the mechanics of microcrack growth and how this is reflected in the continuum response of the material. Both experimental and analytical efforts are in progress. An experimental determination of the relationship between applied stresses and the time-dependent growth of cracks in granite and marble has been established and shown to be consistent with the notion that time-dependent crack growth occurs by the mechanism of stress corrosion. In these experiments, both temperature and moisture were varied.

To apply the experimental results to the problem of time-dependent deformation of brittle rock, a relationship between microcrack behavior and continuum behavior was established through an analytical model based on fracture mechanics and damage theory. The response of rock to various loading histories are being predicted and compared with experimental results.

Current efforts are concentrated on developing a proper definition of damage evolution that includes the interaction of microcracks which occurs when microcrack density becomes large. It is this interaction that results in fault and joint formation prior to failure. Damage rates will be based on test data where the damage accumulation is inferred from acoustic emissions.

C. Creep Response of NaCl at Low Stresses and Temperatures (D.H. Zeuch and W. R. Wawersik)

The objective of this program is to investigate the creep mechanics of sodium chloride at low temperatures and stresses. The creep response of sodium chloride has been studies extensively at temperatures above approximately one-half the absolute melting point, where it appears that dislocation climb is the creep mechanism; however, relatively little work has been carried out at lower temperatures. Such results as are available suggest that the dominant creep mechanism under lower-temperature conditions may be a thermally activated glide or cross-slip process. This in turn implies that creep history and initial substructure may exert a profound influence on the creep behavior of sodium chloride, because recovery is (implicitly) slow.

Work is in progress to conduct creep experiments on sodium chloride single crystals under low stress, low temperature conditions outside the range of any previous testing. Single-stage creep tests will be performed to assess the basic creep properties and substructural evolution of the single crystals. In addition, multistage temperature and stress-changing experiments will be carried out to determine the activation parameters and stress dependence of creep in order to: (1) identify the deformation mechanism(s); (2) quantify the kinetics of recovery; and (3) determine the influence of initial substructure on creep.

A specialized creep frame has been constructed to perform the tests, and a series of cold-working/annealing tests have been carried out in order to develop techniques for the alteration of the initial substructure of the synthetic single crystals. The substructural modification tests also provided preliminary results on the kinetics of recovery of chloride; the apparent activation energy associated with the recovery process is consistent with a cross-slip mechanism at lower temperatures.

Contractor:	SANDIA NATIONAL LABORATORIES Albuquerque, New Mexico 87185
Contract:	DE-AC04-76DP00789
Title:	III. Geochemistry Research
Person in Charge:	W. C. Luth

Scope of Work

Research under this program involves experimental, analytical, and theoretical geochemistry relating to magmatic and hydrothermal processes taking place within the earth's crust.

A. Hydrothermal-Magma Systems (W. C. Luth, T. M. Gerlach, J. C. Eichelberger, and H. R. Westrich)

This research is directed toward developing an understanding of mass and energy transport within and between hydrothermal and magma systems through a combination of field, experimental, and modeling approaches. The research includes electron microprobe analysis of quenched in situ samples of basaltic magma obtained from drilling programs at Kilauea Iki Lava Lake in 1978 and 1981 as part of the Magma Energy Research Program, experimental studies of bubble nucleation and growth in silicic melts, studies of the amounts and kinds of volatiles in young silicic volcanic suites, and the chemistry of volcanic gases including sublimate and condensate fractions. Advanced methods are being developed for use of the fully automated electron probe in geochemical analysis of drill core samples. Computer software is also under development for processing and evaluating large data bases of automated probe analyses with complete propagation of error capabilities. Water CO_2, S, Cl, and F are being determined for a large number of obsidian samples from explosively and effusively erupted young volcanic units at Mono Craters/Inyo Domes and the Cascade Range. These studies have focused on the isotopic composition and amount of water in the obsidian samples as a function of time. The rates of bubble nucleation and growth as a function of water content are being investigated in rhyolitic melts up to 0.5 kbar. Field, analytic, and computer-based studies of volcanic and fumarolic gases are being performed for Vulcano, Usu Volcano, Long Valley, and Kilauea Volcano in an effort to better understand chemical trends during magma degassing.

B. Clay-H_2O Interactions (J. L. Krumhansl)

The ability to predict the course of rock-water interactions at temperatures up to 350°C is critical to a large number of geochemical, geophysical, and energy related problems. To a large degree these predictions depend on a knowledge of the kinetic and thermodynamic constraints governing clay mineral dissolution. This problem has been approached through the use of a Dickson hydrothermal apparatus, and by employing standardized clays. To date the Wyoming bentonite SWy-1 has been subjected to tests of at least two months duration at 200 and 300°C, and in both acidic (pH = 2.1) and neutral solutions. The results of these tests indicate that clay dissolution is highly incongruent, that hydroxide complexing of both aluminum and iron is an important factor in governing the overall solubility, and that when compared to theoretical estimates derived using a Tardy-Garrels type approximation, the clay is somewhat more stable than would have been anticipated. It was also found that run times of at least six weeks were required for the system to achieve steady state; consequently, evaluation of a wide range of clays (of differing compositions) will proceed somewhat more slowly than had been anticipated in the original proposal.

Contractor: SANDIA NATIONAL LABORATORIES
Albuquerque, NM 87185

Contract: DE-AC04-76DP00789

Title: IV. Advanced Concepts

Person in Charge: W. C. Luth

Scope of Work

Research conducted in this program involves exploratory research in several geoscience areas. Typically such research efforts are of a short-term nature and may be oriented toward assessing feasibility of a particular research task.

A. Noble Metals (H. W. Stockman)

The noble metals are designated as strategic and critical minerals by the U.S. government because of their unique properties and energy and defense applications. The goal of this project is to develop an understanding of how noble metals are concentrated and transported by geologic processes. Work has been concentrated on: (1) development of techniques for obtaining high quality analyses of noble metals in rocks and minerals; and (2) experiments with synthetic, noble metal-containing systems, used to interpret noble metal distributions in natural rocks and minerals. Work on analytical methods has involved development of techniques for separation of noble metal-rich Fe-Ni-Cu sulfides from rocks, SEM and electron microprobe analyses of mineral separates and in situ platinum minerals, and development of computer codes for correcting electron microprobe analyses of minute platinum-group minerals. Experimental studies have involved determinations of the solubilities of platinum elements in solid and liquid Fe-sulfides at 1000-1250°C, determination of the Ru-RuS_2 and Ir-Ir_2S_3 sulfur buffers, and investigations in the Pt-S and Os-S systems at high temperatures.

PART II

OFF-SITE

Contractor:	UNIVERSITY OF ALASKA Geophysical Institute Fairbanks, Alaska 99701
Contract:	DE-AT06-76ER70005
Title:	I. Magnetosphere Annihilation and Applications
Person in Charge:	S.-I. Akasofu

Scope of Work

Plasmas in thermonuclear fusion research devices and in space around the earth have much in common. The earth's magnetosphere provides a unique opportunity to study some of the basic characteristics of plasmas. We have learned basic processes associated with the natural dynamo (consisting of the solar wind and magnetosphere) which can generate as much as one million MW. Specifically, University of Alaska researchers are working with thermonuclear fusion groups at the University of Texas, Austin, and the Plasma Physics Laboratory, Princeton University, in applying computational methods developed by them to learn some of the basic characteristics of plasmas in nature. During he last 12 months we have used extensively the electromagnetic codes developed by the fusion researchers in simulating various magnetospheric and solar processes. So far, we have not found any indication that magnetic reconnection can occur explosively (namely, explosive magnetic field annihilation), supplying energy for magnetospheric substorms and solar flares.

University of Alaska researchers are also interested in energy-related geophysical problems in the Arctic region. In particular, they are studying the electric current induced by auroral activity in power transmission lines and in oil/gas pipelines. We have successfully demonstrated that auroral activity causes surges in the protective relay system in power transmission lines. An intense surge will open the protective relay, causing a systematic blackout; blackouts caused by auroral activity are fairly common in Canada where many power transmission lines are rather long. By studying the characteristics of the surges, we are designing a protective relay system which will not be affected by auroral activity. This project is important for the proposed Anchorage-Fairbanks tie line. We have obtained excellent data to study the relationship between the induced current and the protective relay and thus are analyzing them in detail.

In the arctic region, permafrost provides serious obstacles in energy search and oil transport efforts. Thus, the determination of thickness of permafrost is increasingly an important problem. We have an impulse radar (GSSI), loop-loop induction systems (EM-31,-34), audio magnetotelluric systems, and electrical resistivity devices. We made an extensive survey of permafrost in the Prudhoe Bay area last summer and are analyzing the data.

Contractor: ARIZONA STATE UNIVERSITY
Department of Chemistry
Tempe, Arizona 85287

Contract: DE-AC02-80ER10765.A000

Title: Silicate, Aluminosilicate and Borosilicate Melts: Thermal-Chemical Studies by High Temperature Calorimetry

Person in Charge: A. Navrotsky

Scope of Work

High temperature solution calorimetry is used to determine heats of mixing in aluminosilicate glasses and melts. We are focusing on the role of oxide basicity in determining mixing properties along the joins $MAlO_2$-SiO_2 (M = Li, Na, K, Rb, Cs, Mg, Ca, Ba, Sr, Pb) and in determining heats of vitrification and of fusion. These systematics lead to an understanding of effective heats of fusion of diverse components in an aluminosilicate framework. The enthalpies of the substitution $Si^{4+} \rightarrow Al^{3+} + 1/nM^{n+}$ correlate with the field strength z/r of the substituting cation and with the trends shown in TO bond length variations obtained from ab initio molecular orbital calculations. In addition, we have completed study of the system $KAlSi_3O_8$-$NaAlSi_3O_8$-Si_4O_8 and are continuing the modeling of phase equilibria in silicate systems, using experimental heats of mixing and of fusion and models for entropies of mixing. The emphasis is on ascertaining the usefulness of the two-lattice model for the entropy of mixing and in developing more appropriate complex structural entropy models.

In addition, we are beginnning to study other coupled substitutions, especially $Si^{4+} \rightarrow B^{3+} + Na^{+}$ and the substitution of nitrogen for oxygen by reactions such as $O^{2-} \rightarrow N^{3-} + 1/nM^{n+}$. The system Na_2O-B_2O_3-SiO_2 is receiving detailed calorimetric study. These glasses differ from the corresponding aluminosilicates in a systematic fashion.

A pressure vessel for the study of heat contents of hydrous melts in the system $KAlSi_3O_8$-$NaAlSi_3O_8$-Si_4O_8 up 1000°C and 1 kbar has been constructed. It will permit direct study of the thermodynamic properties of glasses and melts containing up to 50 mol% H_2O by drop calorimetry under high pressure.

The data and models are correlated to the structure and physical properties of silicate melts and have potential applications in such diverse fields as geochemistry, magma energy generation, ceramic science, nuclear waste disposal, and reactor safety.

Contractor:	UNIVERSITY OF ARIZONA Tucson, Arizona 85721
Contract:	DE-AC02-80ER10753.A001
Title:	I. Solar Variability: Changes in Figure and Mean Diameter
Person in Charge:	Henry A. Hill

Scope of Work

The objective of this program is to develop and use an indirect diagnostic of changes in the solar constant by monitoring the figure and diameter of the sun over long periods of time. Obtaining reproducible radiometer data over the period of years to decades necessary for a significant study of the changes in solar luminosity constitutes a serious problem; this problem motivated the search for an indirect diagnostic. Such indirect diagnostic of luminosity is offered by measures of changes in the solar shape and mean diameter. Techniques measuring fractional solar diameter changes over approximately 9 hr observing runs to accuracies of $D/D \simeq 10^{-5}$ to 10^{-6} are being used to measure changes over longer, climatically significant time periods. The relationship between this indirect diagnostic and solar constant is being examined.

A. Technical Developments

The success of the program to monitor long term variation in the figure and diameter of the sun depends in large measure on maintaining the stability of the telescope over similarly long periods. To meet this requirement, a focal plane distance calibrator has been designed for the SCLERA astrometric telescope, and its construction and installation is nearly complete. This device consists of a pre-lens diffraction grating; a focal plane stabilized light source; light detectors on the solar detector; and necessary computer and computer related equipment. Hardware is now being installed, and software is starting to be developed. The grating, on low expansion glass, can be placed on the stop of the primary lens and is designed to produce first order diffraction images in the focal plane with the approximate angular diameter of the sun. The light source is a single mode stabilized helium-neon laser. The first order diffraction maxima are imaged on the solar detector and are used to calibrate the angular field. This device will coexist with the Michelson measuring interferometer that measures distances in the focal plane. The Michelson interferometer has been designed and constructed so that the white light fringe can be detected, thus providing a fiducial for day to day comparison of measurements. This system to detect the white light fringe has been in operation since the summary of 1981.

B. Observations

Nearly seventy days of solar diameter measurements have been collected during 1983 with the white-light fringe detecting system in place. Analysis is continuing on the unprecedented quantity of this type of astrometric data. It is expected that these observations contain information on the variation in time of the solar figure and mean diameter and should yield a new measurement of the visual solar oblateness.

C. Theoretical Work

Our ability to infer a particular luminosity change from, for example, an observed change in the mean solar diameter has been quite limited. At present there is a difference of approximately three orders of magnitude between the least and the greatest sensitivity that has been suggested. This large range in the estimates of the sensitivity is, in part, a reflection of the several different physical processes that have been considered potentially important in producing luminosity changes. However, of equal importance have been differences in the treatment of the boundary conditions in the solar envelope. Considerable success has been achieved in refining the treatment of the boundary conditions. Testing of the new theoretical work is currently underway. In addition to the new developments in the theory, information on the ratio of fractional change of luminosity to the fractional change in the solar diameter has been obtained from recent work on global oscillations of the sun. This ratio is found to be about two for variations in the sun that occur over a time scale of hours. To the extent that this ratio is characteristic of the lower frequency, climatically significant variations, these new findings should be quite valuable. These findings will aid interpretation of the results of the solar diameter observations and will aid the testing of SCLERA's theoretical studies know in progress.

Contractor:	UNIVERSITY OF ARIZONA Department of Geosciences Tuscon, Arizona 85721
Contract:	DE-AC02-81ER10842
Title:	II. Rock Deformation in Magma-Hydrothermal Systems
Person in Charge:	Denis Norton

Scope of Work

The goal of this project is to obtain a better understanding of the evolution of stress and strain in fossil magma-hydrothermal systems through the investigation of fracture systematics. Our main objective has been to obtain a data base on the nature of fractures that is sufficient to (a) test previous theoretical studies on the evolution of stress around cooling magmas, and (b) improve techniques for numerical modeling of coupled transport processes around thermal perturbations in the Earth's crust. In establishing this data base, we have discovered several new aspects of fracture topology:

1. In the approximately 30 fossil magma chambers we have studies, which represent a broad spectrum of compositions, ages, exposure levels, and chamber sizes, fractures are oriented with respect to what we infer to have been local stress trajectories present when the magma was emplaced and cooled.

2. Fractures observed in outcrops and shallow drill holes can be used to predict fracture characteristics that will be encountered at greater depths because variations in the abundance and character of fractures as a function of depth are caused by magma-hydrothermal conditions. Weathering processes accentuate the fracture patterns but do not generally cause fractures.

3. Fractures are present today that formed subsequent to the cooling event. Even in one b.y. old systems, these fractures can be readily differentiated from those formed by the thermal event.

4. Fracture extents are much more limited than previously assumed. In addition, the shapes of individual fractures are directly related to fossil stress orientations and relative stress magnitudes.

5. Substantial evidence exists to suggest that fracture topology is a direct consequence of H_2O-rich fluids responding to nonhydrostatic stress conditions.

Because fractures control the response of a rock mass to thermal, chemical, and mechanical perturbations, our research is relevant to engineering design problems related to waste disposal and both natural geothermal and hot-dry-rock reservoirs. We have concluded the following: (1) Thermal perturbations (e.g., waste disposal) embedded in crystalline rocks will very likely cause fractures to propagate away from the heat source at a rate similar to the rate of heat dispersion; (2) Production of fluids from geothermal reservoirs will inevitably lead to deleterious chemical reactions that will ultimately seal the productive wells. This problem can be avoided only by utilizing methods that produce fluids within the constraints imposed by the natural feedback conditions; and (3) H_2O-rich fluids are distributed in virtually all fractures. The intrinsic properties of these fluids and the shapes of the fractures that contain them exert a dominant effect on the bulk modulus of rock. Therefore, the seismic prospecting technqiues used to detect magmas and geothermal resources are inadequate for discriminating between the sheath of fractures around a magma chamber and the magma itself.

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Contractor:	CALIFORNIA INSTITUTE OF TECHNOLOGY Seismological Laboratory, Division of Geological and Planetary Sciences Pasadena, California 91125
Contract:	DE-AT03-83ER13120
Title:	In Situ Stress in Deep Boreholes
Person in Charge:	T. J. Ahrens

Scope of Work

Knowledge of the in situ stress in the earth is important to our understanding of contemporary tectonic, geothermal, and rock-forming processes, and provides information which is required to exploit energy resources and store waste in the earth.

We are developing a new type of stressmeter which employs interference holography and by means of laboratory and field measurements, we are attempting to turn it into a useful geophysical tool.

This development was carried out with a 12" diameter device which is lowered into boreholes and first locks in place. Then a holographic exposure is taken of the borehole wall, a side-core hole is drilled which relieves in situ stress and a second hologram is taken. The resulting interference hologram yields a map of displacement, which is inverted to obtain the 6 components of the in situ stress tensor.

Current Activities (J. Bass, D. Schmitt, and T. J. Ahrens)

We have completed laboratory and initial field tests of this new device, which we believe will become a useful tool in borehole geophysics. Laboratory tests included carrying out measurements on samples, under known prestress, and developing the numerical methods for calculating synthetic interference holograms for inverting field data. In 1983, we carried out a successful series of field tests of the holographic tool at depth in the Union Oil Co. oil shale mine in a series of 12" holes especially drilled for us. We obtained an outstanding set of good results. We have performed a preliminary analysis of these data to yield values of maximum and minimum horizontal stress and stress orientation which agrees well with values obtained by other methods (hydrofracture) in this region by Bredehoeft et al. (1978). These results and the description of the operation of the instrument are currently being described in a scientific paper, "In situ stress measurements with borehole interference holography."

Because most uncased scientific drillholes in the U.S. are 6" or less in diameter, we are currently developing a 5 1/2" diameter field version of the earlier instrument. We expect that this instrument will be compatible with both standard and high temperature 7-conductor borehole logging cable. Many details of design include film transport, optical systems, rotation, locking, orientation transducing, internal pressurization, mud-filtering, and side-hole coring, are being improved as a result of our experience with the 12" "laboratory-field" apparatus. We expect this device could operate initially at depths of several hundred meters using film. With a new indium-oxide coated photoconductor polyvinylcarbozole film which is erasable, and an electronic-optic scanner on-board the apparatus, we expect to eventually provide a television-like display of interference fringes on the surface. With this remote read-out device, we expect that the apparatus will have a depth capability of several km.

A final series of tests of the 12" apparatus is now scheduled for June 1984. After this point we will put all our effort into fielding a 6" device in existing scientific boreholes in S. California and other holes of opportunity.

Contractor: UNIVERSITY OF CALIFORNIA
Department of Geology and Geophysics
Berkeley, California 94720

Contract: DE-AM03-83ER13100

Title Advective-Diffusive/Dispersive Transport of Chemically Reacting Species in Hydrothermal Systems

Person in Charge: H. C. Helgeson

Scope of Work

A phenomenological transport code based on continuum theory is being developed to describe fluid flow and simultaneous chemical reactions representing ion association, oxidation/reduction, ion exchange, and mineral hydrolysis in hydrothermal systems. Mass and heat transfer coupled to reversible reactions by the law of mass action and irreversible reactions described by kinetic rate laws are included in the code. Transport equations representing conservation of mass and energy are solved numerically for transient conditions of fluid flow in porous and fractured media. The fluid flux equation contains an advective term corresponding to Darcy's law and a diffusive/dispersive term based on Fick's first law.

Preliminary tests of the code so far developed include validation of the chemical algorithms used in the code by comparison with the equilibrium speciation and mass transfer program package EQ3/EQ6 developed by Wolery (1979), as modified by Helgeson and Murphy (1983) to include mineral dissolution kinetics. The results of calculations for reaction paths in a closed system obtained by considering a single node in the transport code with appropriate boundary conditions for complex systems involving activity coefficients, aqueous complexes, and reaction products compare favorably with the partial equilibrium model. Furthermore, the computation time is considerably faster, which is indispensible for integrating chemistry with fluid flow. The transport code has also been tested for the case of diffusional mass transfer coupled to reversible precipitation/dissolution reactions by comparing numerical results with the analytical steady-state limit obtained by Helfferich and Katchalsky (1970) for a two-component system. In the transient case considered, the calculations indicate that the zone of mineral precipitation first oversteps the steady-state limit and then dissolves at its boundaries, shrinking in size until steady-state is reached. Multi-mineralic zones were found to move in a complicated fashion before reaching steady-state.

Contractor:	UNIVERSITY OF CALIFORNIA Department of Physics Berkeley, California 94720
Contract:	DE-AM03-76SF00034
Title:	Isotopic Studies on Rare Gases in Terrestrial Samples and in Natural Nucleosynthesis
Person in Charge:	J. H. Reynolds

Scope of Work

This project is concerned with research in rare gas mass spectrometry. The broad objective is to read the natural record that isotopes of the rare gases comprise as trace constituents of natural gases, rocks, and meteorites. In past years, these interests have led to the study of such diverse problems as the dating of rocks, the early chronology of the solar system as revealed by extinct radioactivities, and the elemental and isotopic composition of trapped primordial rare gases in meteorites. In recent years the project has focused progressively more on terrestrial problems.

A. The RARGA Project

The Roving Automated Rare Gas Analysis (RARGA) system is a self-contained, mobile laboratory designed to make precise elemental and isotopic abundance measurements of the noble gases in terrestrial fluids. In 1983 the laboratory was deployed at Yellowstone National Park from late June until early November, acquiring a large data set consisting, for each sample, of an elemental run (He, Ne, Ar, Kr, and Xe concentrations) plus isotopic runs on He, Ne, and Ar. Additionally enough isotopic runs on Xe were carried out to establish that there are no significant ^{129}Xe anomalies in Yellowstone samples and enough calibration runs on air Ne to monitor mass fractionation occurring in the mass spectrometry.

B. Yellowstone Projects

The first completed report on the Yellowstone work is an overview of the November 1983 data set (approximately 80 samples), with emphasis on correlations among the measured parameters in the whole set. The helium-argon data conform well to a plane in $^{3}\text{He}/^{40}\text{Ar}$, $^{4}\text{He}/^{40}\text{Ar}$, $^{36}\text{Ar}/^{40}\text{Ar}$ space, indicating that all samples can be explained as mixtures of three components -- an air component, a crustal component with a $^{4}\text{He}/^{40}\text{Ar}$ ratio of 4.1, and a magmatic component which is as yet not well constrained beyond knowing that

^{3}He/^{4}He exceeds 16 times the air value and that ^{40}Ar/^{36}Ar exceeds 500, in agreement with previously determined limits. The report presents an overview of the neon anomalies (more below), the elemental fractionation patterns (well correlated but not explained), and regional behavior of the quantity $(^3\mathrm{He}/^4\mathrm{He})_{\mathrm{local\ maximum}}$ which falls off quickly to air-like values outside the caldera and has a structure inside the caldera which is reasonably well defined but does not correlate in any simple way with other geophysical parameters.

A brief report is in preparation of an experiment we performed in measuring ^{3}He/^{4}He ratios in soil samples at Yellowstone by the simple practice of inserting the lower, open end of a copper tube, closed at the top, in the soil and leaving it there for two weeks before closing off the air sample it contained. This simple technique detects excess ^{3}He and might be useful in the future for studies of vertical heat flow in Yellowstone.

A project which is well along, but requires analyses of about a dozen more samples collected in 1983 but not yet analyzed, is a study of the noble gas dynamics in Horseshoe Spring, in the Norris Geyser Basin. That spring was sampled extensively at various depths and at various lateral positions in order to understand how convection in that spring, which dissolves air gases at the surface and is fed with subterranean gases at a vent at the bottom, affects the elemental and isotopic ratios observed in the samples. This study, together with some measurements we have made on cold springs in Yellowstone, is a start towards understanding the elemental patterns mentioned above.

Another project which requires additional analyses, currently being carried out with the RARGA equipment, concerns a detailed study of the helium isotopes in Lower Geyser Basin at Yellowstone. Preliminary results indicate varying ^{3}He/^{4}He ratios but correlations with the HCO_3^-/Cl^- ratios in the fluid phase, as might be a reasonable outcome of varying degrees of boiling and steam separation in the fluid there. This work will be reported at the May 1984 meeting of the AGU in Cincinnati.

RARGA obtained the first extensive data set for neon isotopes in Yellowstone and the results are being examined in more detail than was possible in the report on the overview of the data as a whole. There is evidence for both mass fractionation of neon isotopes and occurrence of nuclear anomalies in the isotopic ratios. In our present scrutiny of the data we are concentrating, with some success, on seeing how the isotopic ratios correlate for measurements within given regions in Yellowstone.

C. Well Samples from the Valles Caldera

The RARGA equipment has been used to measure the noble gases from four wells in the Baca field at the Valles caldera and a paper has been completed on the rather simple story those measurements reveal. The sampling was carried out in such a way that the absolute concentrations of the noble gases in the steam were determined quite precisely in addition to the relative elemental and isotopic ratios. We were thus able to show conclusively that the fluid in the Baca wells we sampled are two component mixtures. The origin of these components, and how they correlate with chemical measurements made on these fluids, is discussed in the paper.

D. Noble Gases in Silicate Melts

Data are now being collected in our study of solubilities of noble gases in silicate melts of various compositions and at various temperatures. One of our spectrometer systems has been dedicated to this study and equipped with a pipette of isotopically anomalous He, Ne, Ar, and Xe for precise isotopic dilution measurements on the quenched glasses which are prepared in Carmichael's lab at LBL. Preliminary measurements indicate that there may be surface as well as volume solubilities involved. We are well equipped to check such a possibility with the sensitive laser-microprobe rare gas spectrometer which has been constructed in our laboratory and is now in operation. That instrument is part of our NASA research on extraterrestrial samples, but is available for a few key measurements in this study.

E. New Starts for 1984

We are planning to maintain the momentum in our RARGA project by an annual field deployment. We are beginning to formulate plans for the 1984 expedition. It is important to extend our studies to natural gases so that it is likely that a detailed study of a gas field will be the eventual plan. We will have to add a Cu/CuO furnace to our inlet system for conversion of methane and hydrogen to carbon dioxide and water, but we anticipate that this change in the equipment will be easy to accomplish. Otherwise we are ready to apply RARGA to this new class of problems.

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Contractor: UNIVERSITY OF CALIFORNIA
Department of Earth and Space Sciences
Los Angeles, California 90024

Contract: DE-FG03-84ER13203

Title: Determination of Thermodynamic Functions of Minerals at High Temperature

Person in Charge: Orson L. Anderson

Scope of Work

We are continuing work done in our laboratory for the past three years, measuring the thermal expansivity and elastic constants of certain minerals at high temperature (e.g., well above the Debye temperature of the mineral θ). The new minerals to be measured are NaCl, α-quartz, vitreous silica, TiO_2 and possibly iron (α-phase).

It is proposed to use these new data and the corresponding existing data already measured for MgO, Mg_2SiO_4, and Fe_2SiO_4 to calculate the thermodynamic functions of these minerals into the high temperature range 600°K - 1300°K. These include the entropy, the internal energy, the enthalpy and the free energies.

The thermodynamic functions thus determined would be applicable to a large range of DOE projects including geochemistry, magma energy generation, nuclear waste disposal, and the continental scientific drilling program.

Contractor: UNIVERSITY OF CALIFORNIA AT LOS ANGELES
Department of Chemistry and Biochemistry
Los Angeles, California 90024

Contract: DE-AT03-81ER10965

Title: Adiabats and Gruneisien Parameter at High Temperatures and High Pressures

Person in Charge: R. Boehler, M. Nicol

Scope of Work

The high temperature equation of state may be described by a Gruneisen model for the finite-temperature pressure,

$$P(V,T) = P_o(V) + 3N\, \gamma\, (V) \frac{k_B T}{V},$$

where $T_o(V)$ is the T=0 static lattice pressure. The second term is the high-temperature quasiharmonic approximation to the thermal lattice pressure. The Gruneisen parameter λ (V) is related to the volume change of lattice frequencies. The knowledge of its pressure dependence is of great importance in studies involving high pressures and high temperatures, for example geophysical modeling and shock wave experiments.

Various forms of the volume dependence of γ have been deduced in the past and are frequently used such as for example the Slater model

$$\gamma(V) = -\frac{2}{3} - \frac{V}{2} \cdot \left(\frac{\partial^2 Po}{\partial V^2}\right)_T \left(\frac{\partial Po}{\partial V}\right)_T$$

or simpler forms such as $\gamma \cdot \rho$ = constant. The purpose of our study was to measure the Gruneisen parameter γ at very high compressions (over 50%) and to compare its functional dependence with those shown above. the study includes effects of solid-liquid and solid-solid phase transitions on the volume dependence of γ.

Adiabatic compression measurements were carried out on the highly compressible alkali metals in both the solid and the liquid state. This yields directly the Gruneisen parameter as a function of pressure and temperature. The results for Li, Na K, Rb, and Cs can be generalized in the following form: 1) γ rapidly decreases with compression approaching an asymptotic value of 0.5 at compressions above 30%. This behaviour is significantly different from the Slater or free volume relationships; 2) the pressure dependence of γ in the liquid is essentially the same as in the solid. 3) γ increases by several percent at the liquid-solid transition; 4) at constant volume, γ decreases with temperature. For Cs, both experiment and theory indicate that γ becomes very small as the isostructural electronic transition at 42 kbar is approached and shows a strong increase after the transition.

Contractor: THE UNIVERSITY OF CHICAGO
Chicago, Illinois 60637

Contract: DE-AC02-80ER10763

Title: Water and Magma Bodies

Person in Charge: A. T. Anderson, Jr.

Scope of Work

The emplacement, crystallization and eruption of silicic magmas are important both for the compositional evolution of the crust as a whole as well as for the formation of a variety of ore deposits and geothermal fields. We are continuing development of a new way to determine the pressures of crystallization within such bodies of magma. The new method relies both on the increased solubility of H_2O and CO_2 in silicate melts with pressure and on the preservation of samples of the natural high pressure environment of crystallization as tiny inclusions within virtually rigid crystals. We make wafers of the phenocrysts found in silicic volcanic rocks to expose inclusions of glass for analysis both by the electron microprobe for major elements and by a special vacuum fusion device for H_2O and CO_2. That device has been completely rebuilt with modifications intended to reduce uncertainties in results. A quadrupole mass spectrometer (residual gas analyzer) will be incorporated into the system in order to allow more certain confirmation of the nature of each of the gases present. Uncertainty concerning possible H_2S contribution to apparent CO_2 concentration will be removed. We are also investigating possible use of laser heating of melt inclusions which might help to drastically reduce blanks and sample analysis time. Current work centers on a suite of samples of the rhyolitic Bishop Tuff which includes pumice from the plinian phase as well as each of the major ignimbrite lobes. Analysis of this suite may help reveal change in magmatic vapor pressures with time as the magma body developed prior to the cataclysmic eruption. It may also aid in understanding of dynamic mixing processes within the erupting magma body. The data will also be used to help assess the current state of the magma body(ies) beneath the Inyo domes and Mammoth Lakes.

Stanley Williams joined the project in January of 1984, and the rate of progress increased dramatically.

Contractor: COLUMBIA UNIVERSITY
Lamont-Doherty Geological Observatory
Palisades, New York 10964

Contract: DE-AS02-76E03134

Title: Tectonics of the Eastern Aleutian Arc

Person in Charge: K. Jacob, J. Taber, and L. Sykes

Scope of Work

The geophysical processes associated with subduction and arc-magmatism are investigated in one of the world's major active arc-trench systems. We use primarily seismological methods for this purpose. On an arc-wide basis we compare and synthesize globally recorded seismotectonic information for most of the Aleutians. In the Shumagin Islands section of the Aleutian arc we carry out a very detailed study of this 300-km long arc segment. This in-depth study relies on high-quality data from a digital seismic network for which we operate 14 remote stations linked by telemetry to a central, digital-recording site. This arc segment is a seismic gap for which a 30 to 99% probability has been determined that a great earthquake ($M \geq 8$) will occur within the next two decades. Major research topics presently concern: accurate determination of the geometry and velocities of the interface of the descending Pacific slab against the upper mantle and crust of the overriding North American plate by means of three dimensional seismic ray tracing of direct and converted body wave phases; relative location of the dipping seismic (Benioff-) zone with respect to the slab surface; inversion of local and teleseismic travel time residuals for determination of two- and three-dimensional velocity perturbations associated with the volcanic arc and its magmatic root zone; monitoring of seismic and eruptive activity of Pavlof Volcano and other structures along the volcanic arc, and integration of these results with those from geodetic crustal deformation data to investigate plate coupling and to update the existing estimates of long term probabilities for the occurrence of future great earthquakes by medium- to short-term precursors. Although the study focuses on basic research of the subduction process, immediate applications concern the geothermal energy potential of the Aleutian arc; seismic, volcanic and tsunami hazards reduction to off shore oil lease sale areas that are located directly adjacent to the Shumagin seismic gap and network; other spinoffs concern earthquake engineering, and - perhaps - earthquake prediction. Technical long-term objectives are the sensing and - eventually digital - transmission of high fidelity, wide-dynamic range, seismic ground motion data to the central network recording site capable of resolving the motions of both small and the large earthquakes.

Contractor: HARVARD UNIVERSITY
Department of Geological Sciences
Cambridge, Massachusetts 02138

Contract: DE-AC02-83ER13096

Title: Energetic and Thermochemical Properties of Rocks and Minerals

Person in Charge: J. B. Thompson, Jr. and S. K. Dobos

Scope of Work

Any thorough understanding of the earth's crustal processes and energy budget must take into account the energetics and thermochemical properties of rocks and their constituent minerals, notably their heat capacities and their enthalpies and entropies of transformations. Such thermodynamic data, and physico-chemical models derived from them, are of direct concern in such fields as the extraction of geothermal energy, nuclear waste disposal, terrestrial heat-flow studies, the geochemistry of ore deposits and igneous, metamorphic and sedimentary petrology.

Much of the requisite thermochemical data to handle problems in the above fields is unknown or poorly characterized. We propose to augment the data base for the thermochemical properties of rocks and rock-forming minerals, as well as heterogeneous transformations in rocks involving the appearance or disappearance of mineral phases of a given phase assemblage. Such studies comprise one of the most basic energy-related branches of scientific investigation in the geosciences, and are fundamental to our understanding earth processes and earth materials.

Our calorimetry lab is now complete and fully equipped with three thermoanalytic instruments: (i) a power-compensated differential scanning calorimeter for the temperature range -170 to 725°C, (ii) a heat-flux differential scanning calorimeter for the range 25 to 1700°C, and (iii) a thermogravimetric analyzer for the range 25° to 1200°C, capable of operation with controlled atmospheres from a moderate vacuum to ambient pressure. The instruments may be run semi-automatically, and are interfaced to computers for real-time monitoring, data collection and data reduction.

Contractor: UNIVERSITY OF HAWAII AT MANOA
Hawaii Institute of Geophysics
Honolulu, Hawaii 96822

Contract: DE-AT03-80ER12099

Title: Physical Characterization of Magma Samples

Person in Charge: M. H. Manghnani

Scope of Work

This program involves two areas of laboratory investigation: (1) characterization of physical (density, porosity, and pore size distribution), seismic (V_p, V_s, Q^{-1}), and thermal (conductivity) properties of core samples from Kilauea Iki Lava Lake and (2) viscosity, electrical conductivity, and V_p, V_s, and Q^{-1} of magmatic fluids at elevated temperatures and pressures and as a function of controlled volatile (e.g., H_2O, CO_2) content.

The goals of the proposed research are threefold: (1) to understand how the physical properties of basalts relevant to geothermal exploration and thermal modeling in a volcanically active area are affected by a total environmental system; (2) to investigate interrelationships between the various properties; and (3) to correlate the laboratory data with the models based on theory and field measurements.

Two parts of the proposed work (chemical and mineralogical analyses of Kilauea Iki and other samples, and viscosity and electrical conductivity of magmatic fluids at elevated pressures) are being conducted in cooperation with W. C. Luth at the Sandia National Laboratories.

The physical, seismic, electrical, and thermal properties (diffusivity, conductivity and specific heat) of selected Lava Lake core samples, for which chemical composition and mineralogy have been determined by the Sandia Laboratories (Dr. W. C. Luth), are being interpreted in terms of chemistry, glass content, and mineralogy of these core samples.

We are currently focusing our efforts on the elastic, anelastic, and electrical properties of melts of basaltic and related composition. The temperature and frequency dependence of ultrasonic compressional velocity (V_p) and attenuation (Q_p^{-1}) measurements for various melt compositions are interpreted in terms of viscosity, relaxation time and structure of melt.

The temperature dependence of the melt conductivity of the eight samples from Kilauea Iki samples from different depths is almost the same and follows the Arrhenius equation.

The proposed research, involving close cooperation between the University of Hawaii and the Sandia National Laboratories, provides an impetus to basic energy research needed for acquiring a better knowledge of the fundamental in situ physical properties of rocks relevant to geothermal exploration and to planned projects such as the U.S. Continental Scientific Drilling Program.

Contractor:	LAMONT-DOHERTY GEOLOGICAL OBSERVATORY Palisades, New York 10964
Contract:	DE-AC02-76ER04054
Title:	Fluid Transport Properties of Rock Fracture
Person in Charge:	T. Engelder and C. Scholz

Scope of Work

Our problem is to understand the parameters that limit fluid flow within the crust of the earth. Because the major flow paths are through joints within the crust the rock-water interaction along joints is of most interest to our project. This problem is important to the DOE because the extraction of hydrocarbons and geothermal energy is critically dependent on flow along fractures toward well bores. Yet, the burial of nuclear waste requires conditions which limit or stop the flow of fluid away from the waste repository.

Flow is governed by the mechanical closure of joints as well as the dissolution and precipitation of components within the joints. During the past year our attention has been divided between two projects: 1) the correlation between flow rate and the change in water chemistry along joints; and 2) the closure of random surfaces in contact.

A. Chemistry

Experiments on the correlation between flow rate and the change in water chemistry were run in a triaxial testing machine with confining pressures up to 100 MPa and pore fluid pressures some predetermined fraction of 100 MPa. Temperatures were up to 100 C. The experiments were accomplished by recycling an 80 cc charge through the rock sample (primarily) a quartzite with some impurities and a granite). Usually the sample consisted of a split cylinder to simulate a joint. Samples were taken at predetermined intervals until the 80 cc charge was exhausted.

For very rough joints the flow rate did not change with time as the fluid chemistry approached equilibrium values. At room temperature, 14 days were required for equilibrium between the water and rock. For chemical components such as Ca, Na, K, and Mg equilibrium was approached asymptotically. For a polished joint with smaller apertures equilibrium was established at about the same rate, but the flow rate decreased with time with the rate of decrease slowing after a couple of days. Future work includes identifying the mechanism for this time-dependent flow rate.

B. Closure

The Greenwood-Williamson-Walsh-Grosenbaugh theory describing the elastic deformation of joints has been written in a more general form. We have tested this theory quantitatively in the laboratory. This has been done by comparing joint closure from experiment with joint closure predicted by the theory. These comparisons were made using actual topography data from the surfaces of the joints used in the experiments.

Joint closure experiments were done using fused silica glass as a materials because of its isotropy and its well-known elastic moduli. Joints consisted of saw-cuts whose faces were ground with #220, #120, #80, and #60 polishing grits. Experiments were done where one rough surface was in contact with a flat surface and where two similar rough surfaces were in contact. Maximum stresses reached in these experiments ranged from 7.5 MPa to 10 MPa.

The maximum joint closure at a given normal stress does not, in general, depend solely on the rms height of the surfaces in contact. The amount of joint closure depends more strongly on the shape of the uppermost tail of the probability density function for summits (local maxima) on the surfaces. To compute the surface topography parameters in the joint closure theory using one-dimensional profiles, a model for surface topography must be assumed. The best agreement between theory and experiment is obtained with a model that includes the true skewed nature of the probability density functions associated with the surfaces in contact. For these experiments, the inverted chi squared model for surface topography of Adler and Firman (1981) shows much better agreement with experiment than does the gaussian model of Nayak (1971).

Contractor:	MASSACHUSETTS INSTITUTE OF TECHNOLOGY Department of Earth, Atmospheric, and Planetary Sciences Cambridge, Massachusetts 02139
Contract:	DE-AC02-76ER02534 A0010
Title:	Continental Scientific Drilling Program: The Seismology of Continental Thermal Regimes
Person in Charge	K. Aki

Scope of Work

This program was started as an involvement in two major geothermal projects, namely the Hot Dry Rock Geothermal Energy Development Project of the Los Alamos National Laboratory and the Magma Energy Project of Sandia National Laboratories. The theory and methods developed for interpretation of various seismic experiments conducted at Fenton Hill, New Mexico, and Kilauea Iki, Hawaii, however, found a variety of applications to other geothermal areas and volcanoes, and our research has been evolving into what might be called Volcanic Seismology.

In this program, we are applying the methods of both passive and active seismology to the candidate sites for CSDP, such as Long Valley, Jemez Mountains and Imperial Valley in order to delineate the geometrical and mechanical properties of the geothermal system. We use a set of digital event recorders for collection of high quality data as used in our study of Mt. St. Helens. Our interpretation methods for observed seismic signals from volcanoes and geothermal areas include the effects of seismic wave generation, transmission, scattering, and attenuation in a medium containing fluid-filled cracks.

Major accomplishments in the past year include (1) Development of theory of magma intrusion and volcanic tremor and application to the Mammoth Lakes seismic events, and (2) Determination of frequency dependence of attenuation in the Long Valley. We discovered that Q's and S waves and coda waves in the Long Valley show a unique frequency dependence, which is similar to the Kilauea, Hawaii, region but distinctly different from all other areas so far studied.

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Contractor:	MASSACHUSETTS INSTITUTE OF TECHNOLOGY Department of Earth, Atmospheric, and Planetary Sciences Cambridge, Massachusetts 02139
Contract:	DE-AC02-78ER04972
Title:	Microcracks and Energy
Person in Charge	G. Simmons

Scope of Work

The objective of this project is to develop the scientific basis for the practical utilization of microcracks in DOE energy programs.

Open microcracks control such important properties as hydraulic permeability, electrical conductivity, compressibility, thermal expansion, and the velocities of elastic waves. Healed microcracks provide data on the pressure-temperature-stress history of a rock and may be useful in estimating the properties at the time the healed cracks were open. The potential applications include (1) site characterization for waste repositories; (2) estimation of the changes of permeability of rock in situ due to changes of temperature associated with production in a hot-dry-rocks geothermal system; (3) prediction of the behaviour of certain isotopes in radioactive waste emplaced in granitic rocks; and (4) improvements in the exploration techniques for uranium in crystalline rocks.

We use the petrographic microscope, the scanning electron microscope (SEM) equipped with both high energy resolution backscattered electron detector and imaging system and an energy dispersive x-ray system, and various physical properties measured as a function of pressure to characterize microcracks. The SEM yields information on healed cracks (composition and extent of the minerals that fill formerly open microcracks, extent of healing, and the physical dimensions). Presently open microfractures are characterized with the SEM and also with a high precision technique for the measurement of strain as a function of pressure (differential strain analysis, DSA).

We have examined the mobilization of uranium and rare earth elements in several igneous rocks: Conway and Mount Osceola granites of New Hampshire, Sherman granite of Wyoming and Colorado, the Carnmenellis granite of southwest England, and various granites and contiguous metasedimentary rocks near Augusta, Maine. Several different uranium-bearing and REE-bearing minerals occur in the microcrack in these rocks over extensive geographical areas and vertical depths - at least 250 square kilometers and a vertical extent of one kilometer for the New Hampshire granites. Because thorium-bearing secondary minerals also occur in the same microcracks, it now appears that thorium may have been mobilized along with U and the REEs.

Uranium and REEs were mobilized in the Sherman granite over distances of at least 50 kilometers and vertical extent of 350 meters. They have remained immobile for one billion years. It would appear that this granite provides a guide to the type of crystalline rock for use as a high level rad-waste repository: namely, a granite pluton that has been altered and in which the microcracks are sealed.

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Contractor: UNIVERSITY OF MINNESOTA
Department of Geology and Geophysics
Minneapolis, Minnesota 55455

Contract: DE-AC02-10837

Title Experimental Formation of Chalk from Calcareous Ooze

Persons in Charge: W. E. Seyfried, Jr. and T. Johnson

Scope of Work

The purpose of this project was to determine the chemical and physical changes which occur during the transformation of ooze to chalk. Chalk comprises a large part of the marine carbonate record, and oil is presently being produced from chalk reservoirs. An understanding of the mechanism of chalk diagenesis has implications pertinent to a broad range of problems in geology.

Hydrothermal experiments on three calcareous oozes of different compositions were performed at low water to rock ratios in a flow-through apparatus and a pore fluid sampler apparatus developed at the University of Minnesota. These facilities allow unconsolidated sediment to be compacted and dewatered in the experimental cell. Sediments in the flow-through system were exposed to 300 bars differential pressure, 100 bars pore pressure; those in the squeezer assembly were exposed to 400 bars confining pressure and little pore pressure. Experiments lasted two weeks at 150 C.

The sediments were chosen to reflect the changes in carbonate sediment composition through the Calcite Compensation Depth. The original pore fluid in the oozes was replaced with Mg and $SO_4^=$ free artificial seawater similar to that inferred to exist in chalk formations at depth. The presence of Mg and Sr in the reacted pore fluid and the decrease in pH and Ca concentration reflected Ca-X exchange and the replacement of less stable carbonate phases, while exchange reactions with clays introduced elements such at Si and Fe into the pore fluid. Initial porosity reduction due to compaction was furthered by pressure solution; fragile coccoliths dissolved while solution-resistant forms became more abundant. The sediments in the pore fluid sampler which were exposed to little pore pressure experienced a slightly greater reduction in porosity.

The following conclusions are relevant: 1) The porosity decrease due to compaction and dewatering of calcareous oozes is reinforced by high confining pressure and elevated temperature which produce welded contacts and lithified sediment. 2) The elimination of unstable phases, as reflected by the Ca-Mg exchange and trace element abundances, increases the preservability of the sediment. 3) Trace element abundance in reacted pore fluids can be traced to Ca-X exchange in carbonate phases and exchange reactions with clays. The trace element compositions of reservoir pore fluids and sediments may be useful in the determination of conditions of lithification and diagnetic pathways. 4) Experiments on chalk diagenesis illuminate mechanisms of lithification and porosity retention in chalk reservoirs.

Contractor:	NATIONAL ACADEMY OF SCIENCES/ NATIONAL RESEARCH COUNCIL Washington, DC 20418
Contract:	DE-FG01-82ER12018
Title:	I. Studies in Geophysics
Person in Charge:	Thomas M. Usselman

The Geophysics Research Forum (GRF) of the National Research Council, National Academy of Sciences is conducting a series of Studies in Geophysics dealing with timely scientific and societal aspects of geophysics and the corresponding demand on geophysical knowledge.

The studies include: (1) problem-oriented studies such as demands on geophysical knowledge in connection with climatic variations, fresh water resources, mineral resources, geothermal and other energy sources, natural hazards, and environmental maintenance; and (2) science-oriented studies such as geophysical data, international programs in geophysics, status of developments and opportunities in geophysics, and impact of technology on geophysics. Each study is conducted by a panel selected for the specific purpose. The preliminary findings of each study are presented to the scientific community for comment at a suitable symposium. Two or three studies are expected to be completed each year.

The studies are guided by the Geophysics Study Committee (GSC). Members of the committee are Arthur E. Maxwell (chairman), Colin B. Bull, John C. Crowell, Devrie S. Inriligator, Nicholas C. Matalas, J. Murray Mitchell, V. Rama Murthy, and Ferris Webster; and Thomas M. Usselman, staff officer.

Studies Completed

ENERGY AND CLIMATE (Roger R. Revelle, panel chairman). Published in 1977 (158 pp.).

ESTAURIES, GEOPHYSICS AND THE ENVIRONMENT (Charles B. Officer, panel chairman). Published in 1977 (127 pp.).

CLIMATE, CLIMATIC CHANGE, AND WATER SUPPLY (James R. Wallis, panel chairman). Published in 1977 (132 pp.).

THE UPPER ATMOSPHERE AND MAGNETOSPHERE (Francis S. Johnson, panel chairman). Published in 1977 (169 pp.).

GEOPHYSICAL PREDICTIONS (Helmut E. Landsberg, panel chairman). Published in 1978 (215 pp.).

GEOLOGICAL PERSPECTIVES ON CLIMATIC CHANGE (Preston Cloud, ad hoc committee chairman). Published in 1978 (46 pp.).

IMPACT OF TECHNOLOGY ON GEOPHYSICS (Homer E. Newell, panel chairman). Published in 1979 (136 pp.).

CONTINENTAL TECTONICS (B. Clark Burchfiel, Jack E. Oliver and Leon T. Silver, panel co-chairmen). Published in 1980 (197 pp.).

MINERAL RESOURCES: GENETIC CONSIDERATIONS FOR PRACTICAL APPLICATIONS (Paul B. Barton, Jr., panel chairman). Published in 1981 (119 pp.).

SCIENTIFIC BASIS OF WATER RESOURCE MANAGEMENT (Myron B. Fiering, panel chairman). Published in May 1982 (127 pp.).

SOLAR VARIABILITY, WEATHER, AND CLIMATE (John A. Eddy, panel chairman). Published in July 1982 (104 pp.).

CLIMATE IN EARTH HISTORY (Wolfgang H. Berger and John C. Crowell, panel co-chairmen). Published in December 1982 (198 pp.).

FUNDAMENTAL RESEARCH ON ESTAURIES (L. Eugene Cronin and Charles B. Officer, panel co-chairmen). Published May 1983 (79 pp.).

EXPLOSIVE VOLCANISM: INCEPTION, EVOLUTION, AND HAZARDS (Francis R.Boyd, panel chairman). Published January 1984 (192 pp.).

GROUNDWATER CONTAMINATION (John D. Bredehoeft, panel chairman). Published February 1984 (179 pp.).

Studies in Preparation

Geophysical Data and Public Policy (Michael A. Chinnery, panel chairman). Publication is expected in 1984.

Atmospheric Electrical Environment (E. Philip Krider and Raymond G. Roble, panel co-chairmen). Symposium held June 1983, publication is expected for 1984.

Active Tectonics (Robert E. Wallace, panel chairman). Symposium held December 1983, publication is expected in 1985.

Sea-Level Change (Roger R. Revelle, panel chairman). Symposium is scheduled for December 1984.

Scope of Work

The modular pattern for the Studies in Geophysics was designed to permit selection of the most timely topics to meet the following objectives:

(1) to set forth the current and prospective contributions that the geophysical sciences can make to such concerns of mankind as energy, non-renewable resources, and the environment;

(2) to provide government officials with technological and scientific evaluations that can serve as a basis to assist in decision making in matters involving geophysical research and knowledge, both in policies and programs;

(3) to provide the scientific community a basis for judgments with respect to the development of the basic science of geophysics in the broad sense and with respect to the relative importance to society of the developments within various branches of geophysics.

Contractor:	NATIONAL ACADEMY OF SCIENCES/ NATIONAL RESEARCH COUNCIL Washington, DC 20418
Contract:	DE-FG01-82ER12018
Title:	II. Committee on Seismology
Person in Charge:	Joseph W. Berg, Jr.

Scope of Work

The Committee on Seismology meets twice a year to discuss current topics of major importance relevant to seismology, to review with government agency personnel, in particular, the actions that have resulted from recommendations of the committee and its panels, and to take actions to assure a healthy science which is in a position to provide maximum benefits to the nation and to society. These activities are directed at fulfilling the fundamental mission of the committee, as follows: to maintain an active surveillance of major trends in seismology and of developments related to seismology in allied scientific and technical fields; to provide special studies for government agencies on appropriate subjects or problems; to maintain cognizance of and to provide advice on international seismological activities; to provide advice to government agencies concerning the operation of U. S. Government-supported seismograph networks and data-dissemination facilities; and to coordinate seismologically related activities within the National Research Council, particularly in the fields of earthquake engineering, rock mechanics, geodesy, geodynamics, and geology. Panels are established to conduct ad hoc studies on topics specified by the committee.

Members of the committee are Paul W. Pomroy (chairman), Lawrence W. Braille, C. Allin Cornell, Robert S. Crosson, Ricardo Dobry, Robert B. Herrmann, Thomas H. Jordan, Hiroo Kanamori, Franklyn Levin, David W. Simpson, and Robert E. Wallace; and Joseph W. Berg, Jr., staff officer.

Products

The Committee issued three reports during the contract period as follows: Seismograph Networks: Problems and Outlook for the 1980s (1983); Effective Use of Earthquake Data (1983); and Seismological Studies of the Continental Lithosphere (1984).

Current Activities

The Committee on Seismology is planning to conduct a study and to write a report on Seismic Hazard Analysis which will provide an in-depth review of the statistical and deterministic approaches to the problem.

Contractor: NATIONAL ACADEMY OF SCIENCES
NATIONAL RESEARCH COUNCIL
Washington, DC 20418

Contract: DE-FG01-82ER12018

Title: III. U.S. Geodynamics Committee

Person in Charge: Pembroke J. Hart

Scope of Work

The U.S. Geodynamics Committee (USGC) was established in 1969 to foster and encourage studies of the dynamic history of the earth, with appropriate attention to both basic science and applications. The USGC work is based largely on the recommendations developed by its 17 reporters and their associated groups. In 1976, at the request of the Geophysics Research Board, the USGC began planning U.S. research activities in solid-earth studies in the 1980's. In the following years, the committee devoted a considerable effort to this task; this led to the report, Geodynamics in the 1980's, published in 1980. This report emphasizes the origin and evolution of continental and oceanic crust, the continent-ocean transition, the relation of mantle dynamics to crustal dynamics, and a geodynamic framework for understanding resource systems and natural hazards.

Members of the committee are Jack E. Oliver (chairman), Don L. Anderson, Bruce A. Bolt, Francis R. Boyd, B. Clark Burchfiel, William C. Kelly, David L. MacKenzie, John C. Maxwell, Frank Richter, and David W. Scholl; and Pembroke J. Hart, staff officer.

The list of topics and respective reporters has been subject to continual review and revision, as appropriate. As of December 1983, the list was as follows:

Fine Structure of the Crust and Upper Mantle	J. E. Oliver
Evolution of Oceanic Lithosphere	J. R. Heirtzler
Large Volume Experimentation	R. C. Liebermann
Application of Isotope Geochemistry to Geodynamics	R. E. Zartman
Geodynamic Modeling	D. L. Turcotte
Drilling for Scientific Purposes	F. G. Stehli
Magnetic Problems	C. E. Helsley
Plate Boundaries	J. C. Maxwell
Geodynamic Data -- User's Needs	W. J. Hinze
Geodynamic Data -- Archiving Problems	M. A. Chinnery
Lithospheric Properties	T. H. Jordan
Comparative Planetology	J. W. Head
Continent-Ocean Geodynamic Transects	R. C. Speed
Electrical Properties of the Asthenosphere	C. S. Cox
Coordination of Major Geodynamics-Related Programs	A. R. Palmer
Geophysics Film Series	C. L. Drake

The results of the work of the USGC and reporters have been issued in annual reports (published or unpublished). Highlights are outlined below.

In 1973, the USGC strongly urged the application of seismic reflection profiling techniques to the structure of the earth's crust and upper mantle. Two years later a consortium of four universities (COCORP) began applying this technique. That group has now completed profiles totalling more than 4000 km. This technique has now become a standard tool in investigating the earth's crust and upper mantle.

The USGC strongly supported efforts to develop a continental scientific drilling program. The work of the USGC reporter led to two workshops (1974 and 1978). The report of the 1978 workshop, Continental Scientific Drilling Program (1979), contained the principal conclusion that, with advance planning, a greater scientific return could be obtained through add-on experiments involving a relatively small increased expenditure to the existing large investment in drilling by government and industry. The 1979 report recommended that a national Continental Scientific Drilling Program be organized to facilitate the necessary communication and coordination. As a result of the response by the federal agencies to the report recommendations, a Continental Scientific Drilling Committee was created in January 1980 under the Geophysics Research Board. The USGC actively encourages the development of this drilling program, including add-on investigations in mission-oriented holes and the drilling of holes dedicated to basic scientific objectives.

The reporter for plate boundaries organized cross sections across ancient plate boundaries. Eighteen such cross sections are in preparation of which sixteen have been published; two are in press.

The USGC places strong emphasis on the importance of the transition zone between continental and oceanic lithosphere. The USGC recommended that a series of transects be prepared to set forth existing geological, geochemical and geophysical data along a series of 25 corridors around the North American coast -- from the continental craton across the transition zone to oceanic lithosphere. The transect project began in 1980. It involves eight working groups and more than one hundred people. The working groups met in April 1982 to exhibit and review the results of their work to date; a public exhibit (poster session) and symposium were held at the meeting of the Geological Society of America in November 1982. Preparations of the maps and cross sections was essentially complete at that time. Publication of the resultant maps and section is under way; completion is expected in 1984 or 1985.

The USGC has endeavored to address two main issues regarding geodynamic data: the needs of users and archiving problems. The USGC convened a group in the early seventies to develop new sections of the Guide to International Data Exchange Through the World Data Centers and collaborated with the Committee on Geophysical Data in preparing the solid-earth section of the CGD report issued in 1979. The two USGC reporters for geodynamic data are actively involved with the current study on geophysical data and public policy and the task of modernizing the international Guide.

The USGC took initiative in the mid-seventies to encourage and assist the production of gravity and magnetic maps of the United States; the effort expanded to include North America. Preparation of these maps was strongly supported by the Society of Exploration Geophysicists and federal agencies. The gravity and magnetic maps for the United States were published in 1982 and were the subject of special symposia on applications at the fall 1982 meeting of SExG. Publication of the maps for North America is expected within the next year.

The reporter for electrical properties of the asthenosphere has worked closely with the international committee for a program of the same title. Several meetings have been held with the objective of developing a specific cooperative program between the United States and Canada.

In 1980, the USGC appointed a reporter and associated working group to ensure coordination among major geodynamics-related programs, especially the Circumpacific Map Project, Consortium for Continental Reflection Profiling (COCORP), Continental Scientific Drilling Program, Continent-Ocean Transects, Early Crustal Evolution, Deep Sea and Continental Margins Drilling, Gravity Anomaly Map for North America, LASE, Magnetic Anomaly Map for North America, Tectonic Map of North America, and the USGS Geological Framework Program. An important result: agreement was reached that the major maps will be published on the same projection and at the same scale.

International Lithosphere Program. The International Union of Geodesy and Geophysics and the International Union of Geological Sciences have organized the International Lithosphere Program -- an international program of geodynamics for the 1980's as a successor to the Geodynamics Project, which formally ended in December 1979. The full title of the new program is "Dynamics and Evolution of the Lithosphere: The Framework for Earth Resources and the Reduction of Hazards." International guidance is provided by the Inter-Union Commission on the Lithosphere. The secretariat of that commission is located in the United States; basic support for the practical operations of the secretariat is provided through the USGC. The international program is developing in a manner partly analogous to the new plans of the USGC. In particular, the emphasis has shifted toward the continents and the continent-ocean transition for reasons of scientific and societal relevance, especially in the areas of resources and natural hazards. The USGC serves as the U.S. counterpart to the Inter-Union Commission on the Lithosphere.

Workshop on the Lithosphere. The USGC organized a workshop on problems of the lithosphere which was held in March 1982, in Austin, Texas. The workshop focused primarily on areas of scientific controversy in connection with the lithosphere, with the expectation that this will provide guidance regarding the most productive areas for research in the coming years. Proceedings were published in The Lithosphere: Report of a Workshop (1983).

Future Work of the USGC

1. Identify actions that can be taken in response to recommendations of the reporters.
2. Assess new directions for the committee and new priority topics to which the committee can react directly or via a reporter. This assessment will take especially into account Geodynamics in the 1980's, the discussion at the Workshop on the Lithosphere, the Continental Scientific Drilling Program, the International Lithosphere Program, and recommendations of reports of the Board on Earth Sciences (e.g., Seismological Studies of the Continental Lithosphere; and report of the Committee on Global and International Geology).
3. Address the program of the International Lithosphere Commission (ICL). What action should the USGC take in response to recommendations of the ICL? Can the USGC provide guidance and recommendations for the Lithosphere Commission?

Contractor:	NATIONAL ACADEMY OF SCIENCES/ NATIONAL RESEARCH COUNCIL Washington, DC 20418
Contract:	DE-FG01-82ER12018
Title:	IV. Continental Scientific Drilling Committee
Person in Charge:	Robert S. Andrews

Scope of Work

The Continental Scientific Drilling Committee (CSDC) was established in January 1980 at the National Academy of Sciences-National Research Council to work toward implementation of the recommendations in the report of the July 1978 Workshop on Continental Drilling for Scientific Purposes held at Los Alamos, New Mexico. This report, Continental Scientific Drilling Program (1979), identified a major goal for this program of maximizing the scientific value of current and planned drilling activities of federal agencies and of industry through add-on experiments, and supplementing these efforts with "dedicated" holes drilled for scientific purposes. In 1983 the CSDC became an activity under the newly-established Board on Earth Sciences.

Members of the CSDC are: Francis Stehli (chairman), Charles Bacon, Lawrence Cathles, Charles Drake, James Eidel, Howard Gould, Kate Hadley, John Hermance, William Hinze, Charles Mankin, Jack Oliver, Elburt Osborn, C. Barry Raleigh, Richard Traeger, and Matt Walton; and Robert Andrews, staff officer.

Scientific objectives for the National Continental Scientific Drilling Program are formulated by the panels of the CSDC, six of which currently exist: Thermal Regimes; Basement Structures and Deep Continental Basins; Mineral Resources; Downhole Physical Property Measurements and Fault Zone Drilling; Drilling, Logging, and Instrument Technology; and Sample Curation and Data Management. The CSDC established eight ad hoc task groups to address specific research drilling targets and objectives: Salton Sea Geothermal Field (CA); Valles Caldera (NM); Yellowstone (WY); Creede Mining District (CO); Tonopah Mining District (NV); Red Mountain Mining District (AZ); Southern Appalachians; and Sample Curation Facilities.

A DEW (Drilling Early Warning) NEWSLETTER was established by the CSDC as its mechanism for communicating with the scientific community. This newsletter is distributed on occasion to approximately 2500 researchers in universities and other academic institutions, industry, government laboratories and geoscience administrators, and geoscience societies, and to interested foreign scientists. The most important role of the DEW NEWSLETTER is to announce early in the planning stage important opportunities for add-on investigations to drilling activities of government and industry and encourage collaborative research efforts. It also provides information on the committee's activities, announces important meetings and publications, and serves as a forum for interested scientists to exchange information related to drilling. Nine newsletters were distributed by mid-1984.

In 1980, the CSDC reviewed the scientific plan for add-on investigations to an industry drilling activity in northern Illinois and issued a report entitled Comments of the Continental Scientific Drilling Committee on the Document "Illinois Deep Hole Project -- Preliminary Plan." Research results from this project were published in the 10 September 1983 issue of the Journal of Geophysical Research.

Current Activities

Since the summer of 1983, the CSDC has greatly accelerated its activity. This took place as the result of high interest expressed by the White House Office of Scientific and Technology Policy (OSTP) in providing major incremental funding for a National Continental Scientific Drilling Program for FY 85. Important factors that led to this situation were the publication of the Board on Earth Sciences' report Opportunities for Research in the Geological Sciences and the research briefings to OSTP and other relevant government agencies by the Panel on the Solid Earth Sciences of the Committee on Science, Engineering, and Public Policy.

The CSDC has the goal of fostering the development of a program of maximizing the scientific value of current and planned drilling activities of industry and government agencies through add-on experiments, supplementing these efforts with holes drilled solely for scientific purposes. This goal has been accomplished through newsletters, meeting, and symposia which attempt to inform the scientific community as to the nature of a planned national research drilling program, opportunities for scientists to become involved in drilling efforts that come to the committee's attention, initial primary scientific objectives and highest priority targets for a research drilling program, and providing for an exchange of ideas.

The Panel on Thermal Regimes completed a report (mid-1984) to the CSDC recommending initiation of a new, highly focused scientific drilling program aimed at understanding the roots of hydrothermal systems related to young magmatic intrusions. Primary targets are high level silicic caldera systems of the Valles caldera and the Long Valley-Inyo-Mono region. The importance of the Yellowstone system is discussed in that report; further considerations are being made by a new CSDC task group concerning the viability of this target for the future. The report also recommends making use of add-on investigations wherever possible to further the understanding of the thermal regime of the Salton Trough.

The CSDC learned of an industry drill hole in the Salton Sea Geothermal Field that may provide an opportunity for add-on investigations. The Panel on Thermal Regimes held an open meeting of interested scientists to discuss this opportunity with the principal investigators; the consensus of the group was enthusiastic endorsement of the scientific merit of the plan. The CSDC issued a letter report, Opportunity for Add-on Scientific Experiments in a Republic Geothermal, Inc., Drill Hole in the Salton Sea Geothermal Field, in October 1982. Since that time, the CSDC has followed this project with keen interest and has supported several activities to develop experimental research for this project as it has evolved.

The Panel on Mineral Resources presented a report to the CSDC (mid-1984) recommending major emphasis on drilling to study stacked hydrothermal mineral deposits in four mining districts: Creede, Red Mountain, Tonopah, and Butte.

The Panel on Sample Curation and Data Management prepared a report concerning curation of drilling samples and ancillary data. The impetus for this panel was based in part on results of a DOE-OBES workshop on core curation at Los Alamos in 1981. The report is presently being reviewed by the CSDC for issuance later in 1984. In addition, the CSDC established a task group to outline the specifications necessary for a national drilling sample curation facility. This task group has met, and its report is being prepared for issuance in June 1984.

The Panel on Basement Structures and Deep Continental Basins addressed dedicated drilling based on a number f scientific reports and projects, as well as various compilations of geological and geophysical data. The panel proposed a deep research hole in the southern Appalachians as its highest priority target; a report on its findings is ready for Academy review. The report should be issued by the CSDC in the Summer of 1984. The Panel has held several special information sessions on research drilling at various sectional meetings of the GSA.

The Panel on Drilling, Logging, and Instrument Technology co-sponsored a workshop in late 1983 on diagnostics and drilling to develop dialogue between scientists and the drilling/logging community. Focus for the workshop was on scientific measurements required for research drilling projects recommended by the CSDC. The panel is studying the state of the art in drilling and logging, and will identify advanced technology required to meet scientific needs identified by the other panels of the CSDC.

The Panel on Downhole Physical Property Measurements and Fault Zone Drilling prepared a report identifying the San Andreas fault as the highest priority target to study the processes of active faulting. The panel held a formal symposium on this subject at the AGU 1983 Fall Meeting in San Francisco. This report should be ready for issuance by the CSDC in Summer 1984.

International cooperation and coordination in continental scientific drilling receives continuing attention of the CSDC. The chairman, staff officer and other members of the CSDC are directly involved in the activities of the International Lithosphere Program related to continental drilling, and in discussions regarding bilateral cooperative studies. The CSDC was a cosponsor of the International Symposium on Observatión of the Continental Crust through Drilling, held in Tarrytown, NY, 20-25 May 1984. Members of the CSDC participated in the continental drilling activities at the International Geological Congress in Moscow, August 1984.

Future Activities of the CSDC

The goal of the CSDC will probably change as a national program becomes a reality, with major incremental funding. A group of universities is in the process of forming an organization to manage a national program. Many of the activities of this corporation will be operationally oriented, including decisions on individual projects and funding. Some of the operational activities may be inappropriate for an Academy committee. The future of the CSDC will depend in large part on two factors: (1) the needs of the supporting federal agencies to have an Academy group for oversight of a management organization and for addressing long-term objectives and targets for a national program; and (2) the CSDC's perspective on the ability of the planned management organization to implement the type of the national program called for at the time of the CSDC's establishment.

Contractor:	NATIONAL ACADEMY OF SCIENCES/ NATIONAL RESEARCH COUNCIL Washington, DC 20418
Contract:	DE-FG01-82ER12018
Title:	V. Board on Earth Sciences
Perso. in Charge:	Joseph W. Berg, Jr.

Scope of Work

The fundamental mission of the Board on Earth Sciences of the Commission on Physical Sciences, Mathematics, and Resources is to provide oversight of the solid-earth science activities with the National Research Council, to provide a review of research and public activities in the solid-earth sciences, to assess the health of the disciplines, and to identify research opportunities. This group is to take a leading role in helping to establish scientific policy bearing on larger earth science programs in and on behalf of the United States. A major charge of the Board and its committees is to assess and recommend basic reasearch and its applications to meet national and societal needs.

Members of the Board are William R. Dickinson (chairman), Don L. Anderson, Paul A. Bailly, Thomas D. Barrow, Lloyd S. Cluff, W. Gary Ernst, Michel T. Halbouty, Melvin J. Hill, Carroll Ann Hodges, John Imbrie, V. Rama Murthy, Jack E. Oliver, Stephen C. Porter, C. Barry Raleigh, J. William Schopf, and E-an Zen; and Joseph W. Berg, Jr., staff officer.

The committees of the Board are: Committee Advisory to the U.S. Geological Survey, Committee on Cartography, Committee on Geodesy, Committee on Geological Mapping, Committee on Global and International Geology, Committee on Seismology, Continental Scientific Drilling Committee, U. S. Geodynamics Committee, USNC/Geochemistry, USNC/Geology, USNC/International Geographical Union, USNC/International Union of Geodesy and Geophysics, USNC/International Union for Quaternary Research, and USNC/Rock Mechanics.

Current Program

The Board maintains an awareness of the national, societal, scientific, and technological demands that solid-earth sciences will be expected to meet in the future and takes actions which help to meet the demands. Such actions are taken using existing National Research Council activities where possible. The functions include the following:

1. Identify basic research opportunities and applied research needs.

2. Review new technology and recommend ways by which the earth sciences can best utilize technological advances to provide maximum benefits to society and to the sciences.

3. Assess educational and manpower requirements relating to future national and societal demands on the earth sciences.

4. Provide a mechanism to enhance interrelationships between domestic and international programs, policies, and problems based on the need to recognize that the earth sciences are intrinsically global in nature.

5. Identify problem areas and help provide a means for the dissemination of information to governmental policy makers and the general public on the implications of geological data pertinent to many of our major societal problems.

6. Coordinate activities in the earth sciences with other National Research Council groups having related responsibilities.

7. Provide advice to government agencies on request and at the initiative of the Board.

8. Initiate tasks that stem from and are relevant to the functions given above. The conduct and completion of specific tasks will be achieved through the use of workshops, the appointment of subunits, and/or any other means deemed appropriate and expeditious.

The committees of the Board on Earth Sciences are engaged in all of the functions listed above.

Products

Several reports have been issued by committees of the Board on Earth Sciences. They are: (1) Opportunities for Research in the Geological Sciences; (2) Geology and Our Future: Summary of a Workshop Report; (3) The Lithosphere: Report of a Workshop; (4) Seismographic Networks: Problems and Outlook for the 1980s; (5) Effective Use of Earthquake Data; (6) Seismology of the Continental Lithosphere; (7) Annual Review of U. S. Progress in Rock Mechanics - Rock Mass Characterization; and (8) Hydraulic Fracturing Stress Measurements. The reports are being used by government agencies and the scientific community. One measure of success is that new incremental funding for site selection of continental drilling has been specified by the Office of Science and Technology Policy for FY 1985. This was a recommendation in Opportunities for Research in the Geological Sciences, as well as one of the five research areas identified by the Committee on Science, Engineering, and Public Policy which briefed officials of OSTP and federal agencies.

Contractor:	NATIONAL ACADEMY OF SCIENCE/ NATIONAL RESEARCH COUNCIL Washington, DC 20418
Contract:	DE-FG01-82ER12018
Title:	VI. Geophysics Film Committee
Person in Charge:	Pembroke J. Hart

Scope of Work

The Geophysics Film Committee was established in the National Academy of Sciences to provide scientific guidance for, and to ensure the scientific integrity of, the film series entitled "Planet Earth" that is being produced by PBS station WQED/Pittsburgh in cooperation with the National Academy of Sciences. The series is scheduled for public broadcasting in the 1985-86 season.

The series will include seven one-hour films for broadcasting; the films can be adapted for telecourse and other educational purposes.

The Film Committee's responsibilities include the following tasks:

1. Selection of specific topics and titles for the films in the series. The subject areas for the seven one-hour films are: comparative planetology, solid earth, mineral and energy resources, oceanography and hydrology, climatology and meteorology, solar-terrestrial relations, and a concluding segment on man's impact on the earth.

2. Appointment of a panel for each one-hour film. The basic responsibility of each panel is to assist the Committee and WQED in identifying appropriate scientific topics, scientific activities, opportunities for new filming, and opportunities to utilize existing footage, and to review the film and script as production advances. Thus, each panel will require meetings of the entire panel and of selected subgroups of the panel to accomplish its tasks:

   Each panel (a chairman and approximately five members) will work closely with WQED to explore subtopics for its film and to identify scientists who are at the frontiers in their respective field of study and whose experiments are expected to have a major impact in science.

   The panel will assist in the preparation of the film script.

   Members of the panel may be asked to participate in arrangements for the actual filming.

Each panel will review the film and its script as production progresses.

3. At appropriate stages of production, the Committee will meet to screen and review the seven films for scientific content and accuracy, as well as to confirm that the overall theme of the series has been addressed.

4. The Committee and panels will assist in developing written material to facilitate use of the films for educational purposes.

5. Meetings of the Geophysics Film Committee and its panels have been held or are scheduled during the eighteen-month period of development of themes, and production of the films. In addition, travel by the chairman and staff of the Committee, and by subgroups of the panels, is required.

In 1983, the Committee established a panel to provide guidance in topic selection and production aspects of the solid-earth film. That film entered editing in mid-1984. Corresponding panels for the remaining films have been established; production of those films and associated written material is proceeding in parallel.

Members of the Geophysics Film Committee are: Roger R. Revelle (chairman), G. Arthur Barber, Charles L. Drake, Herbert Friedman, Laurence M. Gould, Thomas F. Malone, John P. Schaefer, Alan J. Shapley, Eugene M. Shoemaker, Walter S. Sullivan, Verner E. Suomi, James A. Van Allen, J. Tuzo Wilson, and Stanley Ruttenberg (senior consultant); and Pembroke J. Hart and Barbara Valentino, staff.

Contractor: UNIVERSITY OF NEVADA
SEISMOLOGICAL LABORATORY
Reno, Nevada 89557-0018

Contract: DE-AS08-82ER12082

Title: I. Investigation of Magma Chambers in the Western Great Basin

Person in Charge: A. S. Ryall

Scope of Work

This research is in support of the Continental Scientific Drilling Site Assessment Program, and is aimed at defining the geometry of magma bodies in Long Valley caldera, California; characterizing seismicity associated with magma injection in the caldera; searching for evidence of other magma bodies in the surrounding region; and supporting complementary investigations by other agencies involved in the Site Assessment Program. Subtasks are described below.

A. Seismic Network Operation

During the last half of 1983 we deployed eight additional seismic stations north and east of Long Valley caldera. The US Geological Survey has concurrently installed 12 new stations in the caldera region. This brings to 33 the number of seismographic stations recording in and around the Long Valley caldera. All of the University of Nevada stations and many of the USGS stations are being recorded on analog magnetic tape at Reno. Station spacing in the southwest part of the caldera is less than 10 km; north of the caldera it is 15-20 km. This network is sufficient to provide at least 20 readings for the location of all earthquakes in the Mammoth Lakes area with magnitude greater than 1.5 ML.

The University of Nevada has developed and tested a digital seismographic system for remote operation. The digital station is a data acquisition system that provides broad-band (0.05-20 Hz), wide dynamic-range (96 dB) digitization of signals from a three-component set of seismometers, and telemeters the data to a central facility where it is continuously recorded. This system has been tested in an experiment in Hot Creek Valley, central Nevada, and three stations are now operating in mine-tunnels at Mina, Bodie, and Washoe Lake. A fourth station is to be installed in the Las Vegas area in the near future. The Bodie and Mina stations will be used to determine spectral characteristics of seismic signals affected by attenuation in Long Valley caldera.

B. Data Analysis

Routine analysis efforts have provided a detailed picture of earthquake distribution through early 1984 and work is in progress to develop a master-event algorithm that will enable us to reanalyze data collected before the dense network was installed in

1982. A New system has been installed that will provide on-line event detection and digitization of the analog seismic signals transmitted to the Reno data facility. This will facilitate analysis of large numbers of earthquakes and will allow waveform analysis of the network data.

C. Interpretation

1. Geometry of the Magma Chamber (C. O. Sanders and F. D. Ryall)

In order to outline the three-dimensional geometry of the Long Valley magma chamber, we have studied propagation effects along 1200 ray paths for nearly three hundred small events around the southern caldera boundary and within the caldera. The primary discriminant for paths through magma appears to be anomalously low (2-3 Hz) signal frequencies combined with the lack of an S-wave. Signal characteristics have been tabulated and mapped for a variety of paths through the caldera and a range of event depths. Two massive magma bodies have been identified in the Long Valley caldera and their geometries have been mapped out in detail in a paper by Sanders soon to be published in the Journal of Geophysical Research. We are also investigating anomalous propagation effects that suggest the presence of magma bodies under Lake Crowley and along the frontal fault system south of the caldera.

2. Magma Injection (A. S. Ryall and F. D. Ryall)

Earthquakes in one small area just east of the town of Mammoth Lakes have tended to occur as intensive swarms having the appearance of spasmodic tremor observed in volcanic regions. Current research is aimed at explaining the localization of this type of activity in the southwestern part of the caldera, and determining the extent to which swarm activity along the southern caldera boundary may represent dike formation.

3. Focal Mechanisms (U. R. Vetter and A. S. Ryall)

In two papers we have concluded that focal mechanisms of earthquakes in the western Great Basin, including the area around Long Valley caldera, vary systematically with depth. Shallow events have strike-slip mechanisms and events at mid-crustal depth have a strong component of normal slip. This variation, taken together with different fault geometries at different depth, is consistent with a process of lithospheric extension involving normal movement on primary faults and the formation of clusters of fissures or dikes due to crustal spreading at shallow depth. We are now reanalyzing regional and worldwide data for several large earthquakes in 1980, to determine whether those events can be explained by a multiple rupture process rather than the fluid injection model recently proposed by US Geological Survey scientists.

Contractor:	RENSSELAER POLYTECHNIC INSTITUTE Department of Geology Troy, New York, 12181
Contract:	DE-ACOZ-81ER10921
Title:	Deep-Burial Diagnesis in Carbonates
Person in Charge:	G. M. Friedman

Scope of Work

The objectives of this research are (1) to gain an understanding of what makes or breaks porosity in carbonate rocks as a result of deep burial, (2) to relate changes in textures of carbonate rocks to depth, and (3) to develop criteria for interpretation of former depth of burial and paleotemperature in strata now at shallower depth. We have adopted three parallel lines of investigation: (1) experimental compaction tests, (2) study of cores, samples, and wireline logs from boreholes of some of the world's deepest hydrocarbon reservoirs, and (3) study of samples from strata now exposed that were formally subjected to great depth of burial and high paleotemperatures.

Compaction tests reveal that ooid samples show appreciable reductions of bulk volume and porosity when squeezed at temperatures and pressures equivalent to overburdens of over 3 to 6.5 km. Ooids develop pressure-solution contacts during experimental compaction. This is consistent with earlier experience that pressure solution is one of the important processes in the overall diagenesis of carbonate sediments. Scaling down of the time factor from millions of years to just a few days of rapidly rising pressures and temperatures might explain the relatively small magnitude of pressure-solution effects that give way to more mechanical grain adjustments through different types of grain breakage. Besides pressure solution, ooids have been deformed plastically developing both longitudinal and concavo-convex contacts. Temperature and salinity of water that saturated the experimentally compacted ooid samples have effects on the nature of grain contacts and styles of grain breakage. Marine water appears to suppress pressure solution and enhances plastic deformation when other experimental conditions remain constant. Higher temperature appears to enhance pressure solution. Change in temperature appears to have little effect on styles of over-burden breakage, but salinity of water has. These changes in ooid grain contacts and ooid breakage are subtle, but consistent in all experiments that have been run and are considered to be significant.

In the deep Anadarko Basin of Oklahoma and Texas carbonate rocks of the Hunton Group (upper Ordovician to Lower Devonian dolostones alone provide porosity (both intercrystalline and moldic). Bulk densities determined by measuring proportions of major minerals (x-ray diffraction) and iron concentration (x-ray fluorescence) permit improved estimates of true porosities and water saturations. We have calculated more porosity and hydrocarbons than expected for select zones. Intervals with less than 4% apparent porosity before correction for iron, actually have 4-10% porosity. Potentially productive intervals have been missed. At depths exceeding 3 km ferroan dolomite and calcite in the Hunton Group carbonates are predictably associated with interbedded argillaceous zones and with the underlying marine Sylvan Shale. The Sylvan Shale is inferred as the source for Mg^{2+} and Fe^{2+} in generating iron-rich dolomite. Increased temperature with depth has been inferred as the predominant factor for dolomitization.

Lower Ordovician carbonate strata in undeformed belts of the northern Appalachian Basin yield depth of burial and paleotemperature data implying a former depth of burial which has not been usually inferred for this area. A study of liquid inclusions in carbonate crystals puts the paleotemperature into the anchizone suggesting a burial depth of several kilometers. In this continuing study we plan to define the depth of burial/orogenic transition zone.

Contractor: RICE UNIVERSITY
DEPARTMENT OF GEOLOGY
Houston, Texas 77251

Contract: DE-AS05-83ER13124

Title: Structural Evolution of Central Brooks Range, Alaska

Person in Charge: H. G. Ave' Lallemant

Scope of Work

The objective of this research program is to acquire a thorough understanding of the evolution of the EW-trending Brooks Range fold and thrust belt in northern Alaska. A NS-trending transect along the Alaska Pipe Line is being mapped in detail at a scale of 1:30,000 and locally at 1:15,000. Available seismic reflection lines and bore-hole data of the northern foothills and the foreland basin are being analyzed to get better vertical constraints.

The Brooks Range consists of Lower Paleozoic rocks which generally are metamorphic and exposed mostly in the southern part of the range, and Upper Paleozoic clastics and limestone and Mesozoic clastic rocks in the northern Brooks Range. The source area of all pre-Middle Jurassic sediments lies to the north: Middle Jurassic and younger sediments have sources to the south. This change of course area has been related to the emergence of the Brooks Range fold and thrust belt in the Middle Jurassic. An older Devonian deformation has been proposed to have affected the Lower Paleozoic rocks and this deformation is related to the Innuitian event of the Canadian Arctic Islands.

In the central Brooks Range lies the so-called Donnerak window. Two models have been proposed to explain the north-dipping thrust faults, north of the window, and south-dipping ones, south of Doonerak. In one model two thrusting events were proposed: the first one south-directed and the second one north-directed. The second model proposes only a north-directed thrusting event. The Doonerak window was supposed to be a basement high in the first model and a basement uplift in the second one.

Detailed mapping during 1983 has shown that only one north-directed thrusting event had occurred, but that the Doonerak window is not a basement uplift, but an exhumed duplex structure. Fieldwork has also shown that the Lower Paleozoic rocks have undergone exactly the same deformational history as the younger rocks; no pre-Upper Devonian structures were found. This may indicate that the Upper Devonian clastic rocks were deposited on the southern flank of a foredeep, too far away from the Innuitian fold and thrust belt to be deformed penetratively.

Structures in the metamorphic rocks of the southern Brooks Range are all correlatable to the ones in the Doonerak window and thus have formed also during the Juro-Cretaceous Brookian event. Slices of ophiolitic rocks are much less penetratively deformed but have also been emplaced by northward thrusting.

Preliminary balanced cross sections incorporating our field data, seismic reflection, and bore-hole data show that it is possible that major structural traps may occur in the central Brooks Range, but that because of their depth would hold only gas.

Contractor: SOUTH DAKOTA SCHOOL OF MINES AND TECHNOLOGY
Rapid City, South Dakota 57701-3995

Contract: DE-AC01-82ER-12050

Title: Thermally Induced Chemical Migration: A Natural Analog Approach

Person in Charge: J. J. Papike

Scope of Work

The major objective of this research is to gain a quantitative understanding of chemical migration in the geologic environment over a range of temperatures and pressures and in diverse geologic media. Contact metamorphic occurrences serve as geologic analogs with the igneous intrusion providing the neat and trace element source, and the country rock the medium through which migration takes place. The specific sites for this study are pegmatite/wallrock interaction zones in the Black Hills, SD. This type of study provides information on chemical migration over geologic times; a time span that cannot be duplicated in laboratory experiments or with presently available calculation procedures.

Key Questions Being Addressed

1. What is the extent of chemical migration under differing geologic conditions, e.g., P, T, composition of solutions, and nature of country rock?
2. What are the relative mobilities of elements of interest, e.g., Cs, Rb, Li, Sr, etc.?
3. What are the mechanisms of migration, e.g., nature of fluid phase, speciation, etc.?
4. What are the mechanisms of retardation, e.g., sorption, equilibrium cation exchange, etc.?
5. What is the partitioning behavior of the elements of interest among the mineral phases in the host rock and migrating fluid phase?
6. What are the mechanisms of fluid and chemical migration through granite complexes? How does this migration manifest itself?

Some Initial Findings from Pegmatite/Wallrock Studies

1. Maximum temperature of country rock was approximately 510-540°C.
2. The migration of Li and Cs has taken place to distances greater than 90 meters. Rb has migrated up to 10 meters.
3. The relative mobilities of Li, Cs, and Rb are: Li > Cs >> Rb.
4. There is no detectable migration of REE, Al, V, Sc, Cr, Hf, U, Th.
5. Sheet silicates are effective trace element traps. Biotite is a much more effective trap as indicated by Kd's for biotite/muscovite pairs: Cs-12.3, Rb-2.5, and Li-4. These partition coefficients agree with experimentally determined coefficients for phlogopite and muscovite and can be rationalized in terms of the crystal chemistry of these sheet silicates. This work is being done in collaboration with J. C. Laul (Pacific Northwest Laboratories), who is conducting the INAA and RNAA analyses.

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Contractor: STANFORD UNIVERSITY
Stanford, California 94305

Contract: DE-AT03-82ER12051.000

Title: I. Mechanism of Zeolite Crystallization and Alteration in Silicate Glasses

Persons in Charge: J. G. Liou and R. J. Donahoe*

Scope of Work

The mechanism of zeolite crystallization is important not only from a theoretical viewpoint, but also in reference to the large field of industrial applications. Despite the importance of zeolites geologically and industrially, relatively little is known about the physiochemical controls on zeolite formation or about thermodynamic properties of zeolites. This project includes the following three major tasks:

A. Experimental Study on the Processes of Zeolite Formation
Our experimental study attempted to 1) examine the effect of solution composition on the composition and structure of some synthetic zeolites in the system Na_2O-K_2O-Al_2O_3-SiO_2-H_2, 2) study the effect of solution composition on the crystallization path of these zeolites, and 3) interpret these observations within the framework of a theory for the crystallization mechanism of zeolites. Three sets of experiments in which phillipsite or merlinoite precipitated from clear solutions were completed. The results showed that at a fixed activity of silica, zeolite Si/Al ratio is a linear function of pH. This dependence is examined in the light of ^{29}Si NMR spectra of the initial solutions. The results are applied to natural zeolite paragenesis and serve to delineate the framework of a comprehensive theory for the mechanism of zeolite crystallization.

B. Synthesis and Characterization of Alkali Zeolites
Zeolites having the structures of phillipsite, merlinoite and gismondine were synthesized from clear solutions at 80°C. Their morphologies, cell parameters and composition were determined and the chemical controls (pH, Na/(Na + K) ratio) on their formation were delineated. Using the experimental results, the occurrence of merlinoite together with phillipsite in saline, alkaline sediments from Searles Lake, California was predicted and confirmed by SEM

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*Present address: Dept. of Geology, Univ. of Alabama, University, AL 35486 observation of selected core samples. Because of their close similarities in physical properties, it is suggested that merlinoite is much more common as an authigenic mineral then is currently realized.

C. Calorimetric Study of Synthetic Zeolites

Low-temperature heat capacities and heats of solution were determined for nine synthetic merlinoites of various Si/Al and Na/(Na + K) ratios. Eleven additional merlinoites will be prepared and their thermochemical properties will be measured. In this way, variation of thermochemical properties as a function of both Na-K and Si-Al mixing can be studied, facilitating the application of the data to natural zeolites.

Contractor: STANFORD UNIVERSITY
Stanford, California 94305

Contract: DE-AT03-76ER71045

Title: II. Porosity with Fluids: Origin and Effects on Physical Properties of Crustal Rocks

Person in Charge: A. M. Nur

Scope of Work

The objectives of this ongoing project are (1) to advance our understanding of physical processes in cracked rocks with fluids; and (2) apply the results to geophysical exploration, reservoir evaluation and the study of shallow crustal processes. Specific current studies are:

1. Seismic Attenuation in Rocks. Measurements of wave attenuation in rocks vs temperature and frequency have revealed that the rheology of the pore fluid, and surface interactions between fluid and solid control wave induced fluid flow in the pores. It appears that these processes dominate mechanism of attenuation in rocks at shallow crustal conditions. The results are being applied to the interpretation of reflection data in oil and gas fields, hydrological exploration, and to seismic models of overpressure zones.

2. Network models of porous rocks with fluids. We have utilized our network model to describe the petrophysical properties of about 50 rocks, and their dependence on overburden pressure, pore pressure, and other variables. The model correctly and accurately predicts the hydraulic, electrical and elastic properties of all the rock studies. Results suggest that the pore space can be characterized as a mix of flat grains in contact, with a wide range of contact shapes. The results are used already in the development of rigorous petrophysical reservoir models, utilizing seismic, core, and log data.

3. Velocity and attenuation in heavy oil sands. We have by now measured the velocities and amplitudes of compressional and shear waves in heavy oil sand sample from the U.S., Canada, and Venezuela as well as sandstones with various hydrocarbons as a function of pressure and temperature. The new results confirm the large decreases in velocity and amplitude upon heating to 125°-150°C. These large changes have been found to be controlled by wave induced phase transformation and/or chemical reactions in the pore fluid. The results are being applied at present in tracking an in situ steam flood for enhanced oil recovery.

4. Pore pressure in the crust. Our numerical model which incorporates hydraulic diffusivity, pressure solution and solution transfer, rock and pore deformation, and tectonic strain rate, is being used

to estimate the tectonic and mechanical conditions under which super pore pressure zones develop in the accretionary wedge in subduction zones; in active fault zones; and during the migration of hydrocarbons from their source rocks to their reservoir rocks. The results show that the main factors which control pore pressure in these situations are the ratio between permeability and pore volume strain rate and the geometry of permeable and impervious zones in the crust. The results of this study will also be used in the evaluation of radioactive waste disposal sites.

Contractor: STANFORD UNIVERSITY
DEPARTMENT OF APPLIED EARTH SCIENCES
Stanford, California 94305

Contract: DE-AT03-84ER12016

Title: III. The Hydrothermal Solubility of Uraninite

Persons in Charge: G. A. Parks and D. C. Pohl

Scope of Work

The equilibrium solubility of uranium (IV) dioxide (UO_2) in aqueous solution is a function of solution composition (pH, ligand concentration, and ionic strength), oxidation-reduction potential, temperature, and pressure. The limiting concentration of uranium in natural aqueous systems depends on these factors as well as adsorption and more complex rock- and soil-water interactions. These constraints must be recognized and accounted for in solution transport and fixation models. The thermodynamic data required to utilize these models and to compute the solubility limit of uranium exist for near-surface conditions of low temperature and high oxidation potential, but data for higher temperatures and pressures is limited both in extent and precision. This is especially true for tetravalent uranium species.

The major thrust of this work is to obtain equilibrium solubility data for stoichiometric UO_2 in the system UO_2-H_2O while varying pH but while maintaining f_{02} conditions at sufficiently low levels to maintain the low oxidation state both in the solid and solution. The temperature range of the experiments is from 100 to 400°C at 500 bars total pressure.

The experimental approach involves reacting spherical, uranium dioxide pellets with solution in Dickson-Gordon hydrothermal apparatus which permits solution samples to be withdrawn into gastight containers at ambient P/T conditions of the experiement. Equilibrium is approached both from over-saturated and under-saturated conditions. The UO_2 solid is characterized both before and after each experiment. The oxygen fugacity (redox potential) is controlled in the experimental apparatus by maintaining a fixed partial pressure of hydrogen within the reaction cell. Attempts to monitor in situ pH at ambient P/T conditions of the experiment have not been successful as it proved impossible to maintain stable electrode potentials for the duration of the experiments. Hydrogen ion activity is now measured at 20°C and extrapolated to the P/T conditions of the experiment by computer.

We have completed a series of fifteen solubility experiments from pH 1 to pH 7 at 200 and 300°C and eleven in the range from 100 to 400°C. Preliminary analysis of the results indicates that total uranium in solution is at least an order of magnitude higher than predicted from thermodynamic calculations using the data base of Lemire and Tremaine (1980) and EQ3/6 (Wolery, 1978). The results show only a very slight increase in solubility from 100 to 300°C.

Our UO_2 is pre-reduced in H_2 at 900°C and NiO in crimp-sealed Pt capsules included in some runs is reduced to Ni metal, verifying that the low f_{02} desired, is achieved. Other investigators have had difficulty in achieving reduction of uranium to U(IV) in solution. We are concerned that persistent surface oxidation of our samples may be responsible for the high solubility and scatter observed.

Because the predicted and measured uranium solubility of UO^2 approaches or falls below the limit of detection of our analytical method (2×10^{-10}M) near neutral pH, we hope to complete the UO_2-H_2O (NaCl - NaOH) system experiments by conducting experiments at high pH to extend and confirm the high temperature solubility data of Tremaine et. al., 1981.

Contractor: STATE UNIVERISTY OF NEW YORK
Albany, New York 12222

Contract: DE-AC02-83ER13013

Title: Thermal Evolution of Sedimentary Basins

Person in Charge: T. M. Harrison

Scope of Work

Our research objective is to assess the usefulness of $^{40}Ar/^{39}Ar$ age spectrum analyses of detrital microcline in providing thermochronological information necessary for reconstructing the thermal evolution of sedimentary basins. Detrital microclines preserve a record of thermal events in the temperature range ~ 100°C to 200°C, depending on length of heating and several mineralogical variables.

During 1983, a study of deep drill core material from the San Joaquin Basin (California) illustrating the feasibility of this approach was brought to completion. We are presently investigating two extensional basins, the Albuquerque Basin (Rio Grande Rift) and the North Sea. Microcline has proved to be very abundant in both areas above depths of ~ 6 km, and $^{40}Ar/^{39}Ar$ analyses reveal small ^{40}Ar diffusion loss gradients in samples from both terranes. Improvements in analytical techniques, especially temperature monitoring, allow very precise diffusion parameters to be calculated from the laboratory Ar loss data and indicate a slightly higher range in activation energy (31-35 kcal-mol^{-1}) than previously thought (~ 30 kcal-mol^{-1}). Temperature histories inferred from these preliminary analyses are generally compatible with the known thermal history giving us confidence that this approach may be used to extract temperature-time information from samples with poorly known burial histories.

In the hope of better understanding the behavior of K-feldspar during a geological heating, we analyzed a suite of samples from the Fenton Hill deep drill holes, thought to have been at temperature for about one million years. However, it appears from our analyses and simple heat flow calculations, that the heating is very recent, on the order of perhaps 100,000 years.

Contractor: STATE UNIVERSITY OF NEW YORK
DEPARTMENT OF EARTH AND SPACE SCIENCES
Stony Brook, NY 11794

Contract: DE-AC02-83ER13112

Title: Geochemistry and Origin of Dolomites

Persons in Charge: G. N. Hanson and W. J. Meyers

Scope of Work

The prime objective of this research is to investigate the geochemistry and petrology of regionally extensive dolomites using radiogenic and stable isotopes, trace elements, and a variety of petrographic approaches. We are applying these approaches to the regionally dolomitized Burlington and Keokuk Formations (Mississippian) in Iowa, Illinois, and Missouri. These data will be the basis for testing detailed quantitative geochemical models, including chemical mass transfer models, to constrain the source(s) and migration path(s) of dolomitizing fluids. A general understanding of dolomites is important because they are significant reservoirs for hydrocarbons and in many regions have acted as conduits for migration of petroleum, brines, and ore-forming fluids.

We are using a wide range of high precision major and trace element analyses (Ca, Mg, Fe, Mn, REE) and stable (C, O) and radiogenic isotopes (Sr, Nd,) within a framework of well-established dolomite and calcite cement zonal stratigraphies as established by cathodoluminescence petrography. In addition, we are investigating fluid inclusions, solid microinclusions, and crystal defect structures in the dolomites. Fluid inclusion work to date has indicated that highly saline fluids and temperatures of 100°C and greater may have been involved in dolomitization. Preliminary solid inclusion work has identified calcite and iron sulfides within the dolomites. The petrographic framework has been extended southward into Missouri and Illinois and shows that the calcite cement stratigraphy and dolomite zonal stratigraphy are regionally consistent over at least 10's of thousands of square miles. Research on petrography and major and trace elements has shown that there are at least three regionally extensive dolomite types which differ from one another in luminescence signatures and in stoichiometry, Fe, and Mn. The REE data for the dolomites show that non-carbonate components have a major effect on bulk samples, and on acid soluble portions. This indicates that dolomite, or diagenetic calcite, must be physically separated from non-carbonates in order to analyze the REE within the carbonate lattice. Results of the REE analyses of dolomites show regional and stratigraphic consistency in absolute amounts and REE patterns. These suggest that REE are essentially immobile during diagenesis. Similarly Nd isotope analyses of dolomites show great consistency whereas Sr isotopes show wide variation, the latter indicating a probable allochthonous source for some Sr. Studies on Sr isotopes and REE on the host limestones are just beginning.

These studies have the potential of developing an integrated approach that could be widely applied to fluid-rock systems, not only for studies of dolomitization, but also for cementation of carbonates and sandstones, for migration of elements related to waste disposal and for the chemical evolution of ore fluids.

Contractor: TEXAS A&M UNIVERSITY
CENTER FOR TECTONOPHYSICS
College Station, Texas 77843

Contract: DE-AS05-79-ER10361

Title: I. Mechanical and Transport Properties of Rocks

Person in Charge: M. Friedman

Scope of Work

Geothermal-energy exploration and exploitation, safe underground isolation of toxic waste, siting of stable nuclear power plants, continental scientific drilling and the problems of earthquake prediction and hazard reduction all require a better understanding of the mechanical and transport properties of rocks and rock masses under confining pressure at high temperature. Our objectives continue to be to learn more about these properties in the brittle and semi-brittle regimes through experimental and observational studies. Our goal is to predict the behaviors of rock masses in which heat is stored naturally or artificially.

A. The Physical Nature of Fracturing at Depth (N. L. Carter)

Having shown that the $\alpha - \beta$ quartz transition affects profoundly the creep rate of Westerly Granite in the transient regime at 200 MPa confining pressure (Ross et al., 1983), we chose to complete our investigations of low pressure static fatigue of the granite by investigating the effects of strain rate. We have thus conducted a series of constant strain rate tests on dry Westerly Granite at 100 MPa argon confining pressure, temperatures from 24 to 500°C, and strain rates ranging from 10^{-4} to $10^{-7}s^{-1}$ (Harris, 1984). As expected, the fracture strength is sensitive to both temperature and strain range over this rate, the failure stress in these brittle and slightly transient tests decreasing with increasing temperature and decreasing strain rate. Strains at failure show a slight decrease with decreasing strain rate at constant temperature. The activation energy estimated for failure processes in the temperature range 24 to 300°C is 14 ± 5 kcal/mole and these are shown to be dominatedly brittle although a combination of rate processes (semibrittle) operate at 500°C. Log time to failure is directly proportional to -log strain rate, virtually independent of temperature in the 24 to 500°C range studied. An analysis of the creep results of Kranz et al. (1982) and Bauer (1983) over the temperature interval 200 to 600°C reveals an identical result.

Having completed our work on low pressure-moderate temperature static fatigue of Westerly Granite in the dominantly brittle range and on high-pressure-moderate-to high-temperature deformation, in the solid pressure medium equipment dominantly in the steady-state-semibrittle to ductile regime, we are currently beginning an investigation of the creep behavior at intermediate physical conditions, supported by DOE/BES, Contract DE-F605-84-ER13216. These experiments, to be conducted at constant strain rates in the range 10^{-4} to $10^{-8} s^{-1}$ at 400 to 800°C at argon confining pressures of 800 MPa (entirely in the α-quartz stability field) on both nominally dry and induced seawater pore pressures to 500 MPa, will permit a thorough physical understanding of the evolution from elastic-brittle, through transient (work-hardening)-semibrittle to steady-state-semibrittle-ductle flow.

B. Fracture Permeability of Crystalline Rocks as a Function of Pressure, Temperature, and Hydrothermal Alterations (B. Johnson)

The long-term objective is to measure and understand the variation of fracture permeability of several typical crustal crystalline rocks as a result of hydrothermal reaction with through-flowing aqueous fluids at temperatures to 300°C, fluid pressures to 20 MPa, and confining pressures to 100 MPa. Experiments are designed to evaluate the relative importance of dissolution and secondary mineral formation on permeability changes. Complementary experimental and theoretical studies aim at assessing the role of elastic and inelastic deformation of fracture-surface asperities upon changes of fracture permeability.

A servo-controlled permeability system has been designed and built that allows measurement of permeability using either a continuous flow method or transient pulse method with highly corrosive aqueous fluids at elevated temperatures. In a continuous flow mode, one can control either the flow rate (to 1 ml/day) or differential fluid pressure.

Early experiments have focused on determining how dissolution modifies fracture surfaces of quartzite and hence changes fracture permeability. Experiments indicate pronounced changes occur and that intragranular and intergranular (grain boundary) cracks, pores, and tubules play the dominant role in the dissolution modification of surface roughness, with grain-boundary widening being especially prominent. The experiments also clearly show that cutting and grinding induced microcracks markedly influence the early stage of fracture-surface modification and that one must give careful consideration to their influence when performing permeability experiments on "artificial" fracture surfaces (e.g., saw cuts) in a chemically reactive fluid environment.

C. Mechanical Properties of Rocks at High Temperatures and Pressures (M. Friedman and J. Handin)

The deformation of room-dry and water-saturated Westerly Granite is being investigated at confining pressures between 20 and 200 MPa and temperatures between 25 and 900°C, in order to evaluate (1) time-dependent effects of strength and strain to failure, (2) frictional strength of bare-rock surfaces, and (3) effect of temperature on tensile strength, i.e., the possible thermal activation of the tensile fracture process.

With regard to our preliminary conclusions about borehole stability in crystalline rocks at low confining pressures but high temperatures, we note that (a) the creep-rupture strength of granite is only about 20 percent below the short-time triaxial strength so that for geotechnical applications and failure in compression the effect of time may be ignored; (b) results from twenty-four frictional sliding tests indicate that the frictional strength of smooth surfaces of granite is only about 50 percent of the intact strength; and (c) results from twenty-two triaxial extension tests show that the tensile strength of granite drops from about 10 MPa at 25°C to sensibly zero at 800°C. This suggests that fracture is in fact a thermally activated process and it emphasizes the necessity to keep borehole-pressures du'ing drilling less than the least compressive principal stress in the rock mass to avoid hydraulic fracturing. The next steps in this study are to (1) study the textures and fabrics of tensile fracture surfaces and of precursive side cracking in Westerly Granite specimens to detect changes, if any, with increasing temperature (and decreasing strength), (2) extend our triaxial-extension testing to other rock types (e.g., basalt and pure quartzite) to further study tensile strength changes with temperature and the thermal activation of fracture, (3) extend our sliding friction work to these same rocks, and (4) look into the effects of water, surface roughness, and mineralization on the frictional properties of pre-existing fractures (joints). With regard to (3), we would expect the strength reduction observed for smooth rock surfaces to decrease, perhaps vanish, when rough and mineralized natural fracture surfaces are tested. If so, we may still find a pressure and temperature regime in which a jointed rock mass can be modeled solely as a continuum.

Contractor:	UNIVERSITY OF TEXAS AT AUSTIN DEPARTMENT OF GEOLOGICAL SCIENCES Austin, Texas 78712
Contract:	DE-AS05-83ER-13119
Title:	Investigation of a Fossil Geothermal System, Hamblin-Cleopatra Volcano, Clark County, Nevada
Person in Charge:	D. S. Barker

Scope of Work

In the Lake Mead area, Southern Nevada, a Miocene high-potassium andesite-quartz latite stratovolcano was segmented by strike-slip and normal faults. Erosion and faulting have exposed the entire volcanic succession, the intrusive core, a radial dike system, and sedimentary and volcanic rocks predating and postdating the stratovolcano. Mapping at a scale of 1:12,000, completed before this contract began, permits estimates of the proportions of igneous material that formed intrusive bodies, lava flows, and reworked debris during growth of the cone. Such data are essential in constructing better models of subvolcanic geothermal systems.

Mineralogical and chemical changes were imposed on the volcanic and intrusive rocks by convecting groundwater. The exhumed core of hydrothermally altered rocks represents a fossil geothermal system. Alteration increases toward the focus of the radial dike system, and most rock units can be sampled in fresh as well as in variously altered states; thus the compositional changes induced by alteration can be distinguished from those produced by magmatic processes. Field observations of fracture aperture and spacing, and laboratory measurements of porosity, are being used to quantify the hydrologic characteristics of the rock units. Mineralogical and trace element changes, and variations in isotopic ratios of oxygen, hydrogen, and carbon, will be related to permeability and porosity, as well as to sample locations, permitting reconstruction of flow patterns and temperature gradients in this geothermal system.

The first stage of this contract has been to investigate the magmatic processes that accompanied and powered the hydrothermal convection. Major-element and trace-element (Rb, Sr, Y, Zr, Nb, Ni) analyses have been completed on 24 whole-rock samples from stratigraphically well-located lava flows, to document changes in magma composition through time. More than 800 electron probe analyses have been made on phenocryst phases. Bimodalities in compositions of orthopyroxene, clinopyroxene, plagioclase, magnetite, and ilmenite, as well as reverse zoning in plagioclase and cyclicity in trace element concentrations, indicate magma mixing during repeated replenishment of the shallow magma chamber that fed the Hamblin-Cleopatra Volcano. The most highly fractionated liquid (quartz latite) was erupted early in the history of the volcano, and was followed by an oscillatory trend toward more mafic liquids (andesites).

Contractor: UNIVERSITY OF TULSA
Tulsa, Oklahoma 74104

Contract: DE-F605-84EF13220

Title: Stability of Natural Gas in the Deep Subsurface

Persons in Charge: C. Barker and N. Takach

Scope of Work

We have continued to investigate the stability of natural gas in the deep subsurface using a combined theoretical and experimental approach. The stability of natural gas in reservoirs of various mineralogies is being calculated using a computer program that finds the minimum free energy in multicomponent (up to 70), multiphase (up to 30) systems for conditions corresponding to temperatures and pressures down to 40,000 ft (12 km). Equilibrium compositions have been computed for low, average, and high geothermal gradients; hydrostatic and lithostatic pressures; and with or without graphite. Graphite is present when deep gases are generated by cracking oil but is absent if reservoirs were originally filled with methane alone. Calculations have been made for sandstone reservoirs with various amounts and combinations of feldspars, clays, carbonate cements and iron oxides, with and without graphite; and for limestone and dolomite reservoirs with various combination of clays, iron minerals, anhydrite, and sulfur, again with or without graphite. Natural gas shows considerable stability in sandstone reservoirs under most conditions, but its concentration in deep carbonates is much more variable and tends to a hydrogen sulfide-carbon dioxide (H_2S-CO_2) mixture, except when an appreciable concentration of iron is present. Hydrogen is present at the one to two percent level for most lithologies. Preliminary calculations have been made for igneous reserviors.

The thermodynamic predictions can (in principle) be checked by direct analysis down to the depth limit of available samples. To avoid the severe problems of contamination and gas loss during sample retrieval, the gas trapped in fluid inclusions in late stage cements is being used. The fluid inclusions are opened by heating in a vacuum system that forms the inlet to a computer-controlled, gas scanning mass spectrometer. In the past year the analytical system was moved to a new building and rebuilt with an improved configuration. A signal conditioner has been added to the computer hardware so that the mass spectrometer response for minor components can be preferentially amplified. In addition, improved software plus additional memory now allows evolution of several individual gases (H_2O, CH_4, H_2S, etc.) to be monitored continuously while at the same time analyzing gases from bursting individual fluid inclusions. Up to 400 inclusions can be analyzed in a single run with a typical sample size of 10 mg. Inclusions have been analyzed in both silica and carbonate cements and show a variety of compositions depending on environment. Often different generations of inclusions in the same sample will show quite different compositions. While shallow samples often show a range of hydrocarbon samples from below 20,000 feet have been range from a major component to traces in including hydrogen sulfide. The gas compositions are being [illegible] calculated using the thermodynamic program.

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Contractor: UNIVERSITY OF WISCONSIN
DEPARTMENT OF GEOLOGY AND GEOPHYSICS
Madison, Wisconsin 53706

Contract: DE-FG02-84ER13184

Title: Thermal Stress Microfracturing of Granite

Person in Charge: H. F. Wang

Scope of Work

The mechanical and hydrologic response of rock masses to heat is an important basic research area especially relevant to predicting the long-term behavior of a geologic repository for radioactive waste. Such research also has applicability to natural heat sources such as the effect of a magmatic intrusion on the hydrothermal system in country rock, or to the production of geothermal energy.

High temperatures dramatically reduce the elastic moduli of granites, even under high confining pressures. This effect is attributed to microcracks created by internal thermal stresses. A spherical inclusion model has been used to predict whether a given change in temperature or pressure will introduce a tensional crack between a mineral constituent and the rock matrix. We are able to predict crack densities, and hence elastic moduli as a model rock is subjected to changes of P and T. The results are critically dependent upon the P,T path to which the rock is subjected. Comparisons are made for the case in which the rocks are heated only at maximum pressure, then compressed isothermally. The comparisons are quite close for three granitic rocks, but underestimate the crack densities of quartz-free gabbro and basalt.

A detailed description of thermally-produced crack porosity is important to improvement of the crack model. High resolution crack porosity data will be obtained for several granites which have been heated to high temperatures at high confining pressures. The crack characterization will be by differential strain analysis and by direct observation with the optical microscope and the scanning electron microscope. Given the crack porosity data, it should be possible to refine a differential thermal expansion model to reflect the observed distributions and types of cracks within different minerals.

This project is joint with Lawrence Livermore National Laboratory. The microcrack data and modeling described above will be related to physical property measurements made there. These data will include elastic wave velocities, electrical conductivity, and permeability as functions of pressure and temperature. Consideration will be made of different pressure, temperature paths.

Contractor: WOODS HOLE OCEANOGRAPHIC INSTITUTION
Woods Hole, MA 02543

Contract: EG-77-0204392

Title: Organic Geochemistry of Outer Continental Margin and Deep Ocean Sediments

Persons in Charge: J. M. Hunt and J. K. Whelan

Scope of Work

The objective of this program is to develop a better understanding of the processes of hydrocarbon generation and migration in coastal and offshore sedimentary basins as an aid in predicting favorable exploration areas for petroleum. Our research is concentrating on the light hydrocarbons in the C_1 through C_{15} range since these hydrocarbons are not formed by living processes except for methane and possibly some ethane. Also, these are the hydrocarbons that migrate most easily by diffusion, solution in pore waters or in the oil and gas phases.

The stratigraphic intervals generating the $C_1- C_{15}$ hydrocarbons have been identified in shale sections of four wells in the Gulf of Mexico and four wells on the North Slope of Alaska. Migration of these hydrocarbons has been followed through sediments of varying lithologies and organic richness. Methane and ethane were found to migrate over far greater vertical distances from their source beds than the C_{3+} hydrocarbons over tens of meters in 80 million years in fine-grained sediments. Lateral and vertical migration does appear to occur within the oil generation interval (~100°C) with the smaller molecules migrating first.

An ion trap detector is being added to the pyrolysis apparatus in order to monitor evolution of various gases during the pyrolysis process. It is hoped that specific gases will give clues as to both the type and maturation state of the kerogens. The headspace analysis for light hydrocarbons has been modified by changing to a 100 m fused silica glass capillary column. It has been found that 10% PhMe silicone gives as good separation as the standard HHK column in the C_5-C_8 range. The advantages of the fused silica column over HHK are due to its much higher temperature capability (350°C as compared to 50°C for HHK). This will enable the detailed hydrocarbon analyses to extend to a higher range.

We are also analyzing gases of Deep Sea Drilling Project sediments from the Gulf of Mexico in order to learn more about the initial stages of light hydrocarbon migration in sediments.

Future work on this project will concentrate on mechanisms, directions, and distances of oil and gas migration, the depth and extent of gas generation and the potential hydrocarbon resources of the outer continental slopes and rises.

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Contractor:	XDATA CORPORATION 6124 N. Chester Avenue Indianapolis, Indiana 46220
Contract:	DE-AC02-82ER12054
Title:	Computerized Underground Image Reconstruction
Person in Charge:	K. A. Dines

Scope of Work

The general aim of this work is to develop computer-aided imaging techniques for visualizing the subsurface geology. Work is currently centered on the investigation of computed reflection tomography for application to underground imaging. The imaging technique is based on a line-integral measurement model for incoherent acoustic backscattering from elliptical integration paths through a two-dimensional underground cross section. Computer simulation results have been produced illustrating the image quality obtainable for the case of a linear surface array of sources and receivers. Test results include images of layered structures, lines, and point reflectors obtained by an iterative reconstruction technique applied to simulated data.

The method is aimed at near surface imaging situations in which high resolution is required for the detection of buried objects, fractures or other signficant scattering features.

Computer software has been designed, implemented, and tested for the forward (data generation) problem and the inverse (reconstruction) problem in computed reflection tomography using a linear array. The initial results indicate that good depth and lateral resolution is obtainable for depths up to one half of the total array (aperture) width. Below this depth, the lateral resolution deteriorates rapidly so that only a horizontally layered representation can be obtained.

The reflection tomography model, as implemented for the general case, does not assume any particular center frequency for pulse-echo probing, and can therefore be scaled to fit particular array lengths and compatible frequencies. The basic data collection and reconstruction model is strictly valid only under simple assumptions for the backscattering process. These assumptions are: (1) the velocity of sound in the medium is essentially constant, so that errors in round-trip delay time and the departure of the wavefronts from circular arcs are small compared to the desired image resolution; (2) attenuation due to adsorption in the medium is either known or is negligible; (3) attenuation due to scattering is neglected, and there are no second-order scattering effects; and (4) the scattering is assumed to be isotopic.

Continued work on this problem is aimed at investigating the effects of noise and quantifying the relationship between array parameters and resolution as a function of position in the image plane.

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Contractor: YALE UNIVERSITY
DEPARTMENT OF GEOLOGY AND GEOPHYSICS
P. O. Box 6666
New Haven, Connecticut 06511

Contract: DE-AS02-76ER10455

Title: Opening Mode Crack Growth in Rock

Person in Charge: Robert B. Gordon

Scope of Work

The objective of this research is to develop an understanding of the fracture strength of brittle rock that can be used in the solution of engineering design problems and in the field. The specific energies for crack initiation and propagation in nine different types of rock have been measured in the laboratory. The experiments show that, because of the non-linear elasticity of rock, the measured fracture energy depends on the way in which the test specimen is loaded. Hence, a standardized test procedure is needed to obtain data that show the differences in fracture energies that are due to differences in structure and composition of rock. The fracture toughness is found to depend primarily on the preexisting microcrack network in the crystalline rocks and is less influenced by mineralogical makeup and texture. Rock which is relatively free of microcracks (such as quartzite), or in which cracked or porous material is organized in nearly continuous sheets (such as limestone), or which has a very high concentration of microcracks (such as marble), tends to have a low fracture energy. High fracture energy is found when rock contains a microcrack network that permits development of multiple, partially completed, fracture paths.

The micromechanical processes that control the fracture energy and the structure of the fracture surfaces in rock are being studies by direct observation of crack growth under the microscope. Highly polished specimens are used in a small but stiff loading frame that permits stable crack growth. Successive loading-unloading curves are recorded and used to compute the energy consumed in each observed increment of crack extension. The size and structure of the process zone formed by the advancing crack is found to be sensitive to the microstructure of the rock. The results are being used to interpret the dependence of fracture energy on crack length and rock structure which was observed in the tests on large specimens.

GEOSCIENCES RESEARCH (ERDA/DOE)
Historical Summary/Off-Site
(Operating Funds - Thousands)

Institution (PI)	FY 1975	FY 1976	FY 1977	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984
U/Alaska (Akasofu)	$ 41	$ [illegible]	$ 79	—	$ [illegible]	$ [illegible]	$ [illegible]	$ 113	$ 117	$ [illegible]
U/Alaska (Pulpan)	79	32	42	[illegible]	113	87	70T	—	—	—
U/Alaska (Kienle)	90T	—	—	—	—	—	—	—	—	—
U/Arizona (Hill)	—	—	—	—	—	91	[illegible]	[illegible]	101	56
U/Arizona (Norton)	—	—	—	—	—	—	[illegible]	[illegible]	[illegible]	—
Arizona State (Navrotsky)	—	—	—	—	—	35	62	[illegible]	123	—
Aspen Institute (Roberts)	—	—	—	48	57	71T	—	—	—	—
Brown U (Hermance)	—	—	—	—	[illegible]	140	104	105	333	—
Cal Tech (Ahrens)	—	—	—	—	—	—	—	—	72	81
U/California-B (Reynolds)	63	130	127	[illegible]	127	[illegible]	144	[illegible]	[illegible]	[illegible]
U/California-B (Helgeson)	—	—	—	—	—	—	—	—	204	—
U/California-D (MacGregor)	—	—	—	71	61	23	—	—	—	—
U/California-LA (Warren)	46	[illegible]	41	[illegible]	100	107	121	NFXT	—	—
U/California-LA (Boehler)	—	—	—	—	—	—	46	NFX	[illegible]	[illegible]
U/California-LA (Anderson	—	—	—	—	—	—	—	—	—	[illegible]
U/California-LA (Kennedy)	[illegible]	[illegible]	[illegible]	[illegible]	72	72T	—	—	—	—
U/California-SD (Craig)	—	—	—	—	—	—	—	—	—	35
U/Chicago (Anderson)	—	—	—	—	—	64	NFX	38	[illegible]	NFX
Columbia U (Fairbridge)	75T	—	—	—	—	—	—	—	—	—
Columbia U (Jacob)	190	200	240	[illegible]	274	312	318	318	[illegible]	[illegible]
Columbia U (Engelder)	—	65	62	76	100	140	100	[illegible]	[illegible]	—
Columbia U (Walker)	—	—	—	—	—	—	—	—	—	73
Ft. Lewis College (Ellington)	—	2	—	—	—	—	—	—	—	—
Harvard U (Thompson)	—	—	—	—	—	—	—	—	372	—
U/Hawaii (Manghnani)	—	—	—	—	—	—	—	[illegible]	[illegible]	[illegible]
Headquarters Services	—	—	—	—	—	—	—	6	1	3
Indianapolis Ctr. for Adv. Research (Dines)	—	—	—	—	—	[illegible]	64T	—	—	—
U/Minnesota (Johnson)	—	—	—	—	—	—	[illegible]	57	NFXT	—
MIT (Aki)	35	100	130	113	142	102	[illegible]	161	[illegible]	147
MIT (Simmons)	—	—	—	[illegible]	100	[illegible]	[illegible]	[illegible]	[illegible]	113
NAS/NRC (U.S. National Comm. Geochemistry)	—	—	—	—	—	—	19	22T	—	—
NAS/NRC (Studies in Geophysics)	4	4	4	—	6	27	29	[illegible]	—	30
NAS/NRC (Comm. on Seismology)	—	9	9	9	9	9	10	14	—	10
NAS/NRC (Geol/Materials Sci. Study)	—	—	—	—	14	—	10T	—	—	—
NAS/NRC (Geol. Sci. Board)	—	—	—	—	—	—	—	13	—	10
NAS/NRC (Geodynamics Comm.)	—	—	—	—	16	70	30	[illegible]	—	[illegible]
NAS/NRC (Cont. Sci. Drilling Comm.)	—	—	—	—	—	[illegible]	70	[illegible]	—	[illegible]
NAS/NRC (Geophys. Film Comm.)	—	—	—	—	—	—	—	—	—	20
Naval Weapons Support Center (Tanner)	—	6	—	—	—	—	—	—	—	—
U/Nevada-R (Ryall)	—	—	—	—	—	—	—	76	87	[illegible]
CUNY-Q (Schreiber)	—	—	—	—	—	—	63	81	48	—
SUNY-A (Dewey)	—	—	—	—	—	—	[illegible]	—	NFXT	—
SUNY-A (Harrison)	—	—	—	—	—	—	—	30	130	—
SUNY-SB (Papike)	—	—	—	—	51	[illegible]	[illegible]	—	—	—
SUNY-SB (Hanson)	—	—	—	—	—	—	—	—	112	118
NOAA (Donnelly)	—	—	—	6T	—	—	—	—	—	—
U/Oregon (Weill)	—	—	—	—	—	—	—	—	100	[illegible]
Oregon State (Fehler)	—	—	—	—	—	—	—	28T	—	—
Pennsylvania State U (Martin)	—	—	—	—	—	[illegible]	[illegible]	NFXT	—	—
Pennsylvania State U (Given)	—	—	—	—	—	—	—	—	—	100T
Princeton U (Hollister)	—	23T	—	—	—	—	—	—	—	—
Rice U (Baker)	—	—	—	—	—	16	—	7	—	—
Rice U (Ave Lallemant)	—	—	—	—	—	—	—	—	130	121
RPI (Friedman)	—	—	—	—	—	—	91	[illegible]	[illegible]	—
SMU (Blackwell)	—	—	—	—	—	—	84	70T	—	—
S. Dakota Sch. M & T (Papike)	—	—	—	—	—	—	—	67	[illegible]	130
U/S. Florida (Sackett)	—	—	—	—	—	—	34T	—	—	—
Stanford U (Liou)	—	—	—	—	—	—	—	34	46	NFXT
Stanford U (Nur)	—	[illegible]	[illegible]	104	147	140	140	128	160	172
Stanford U (Parks)	—	—	—	—	—	—	—	57	[illegible]	[illegible]
U/Texas-A (Barker)	—	—	—	—	—	—	—	—	[illegible]	—
Texas A&M (Friedman)	—	—	—	—	63	[illegible]	262	[illegible]	201	[illegible]
Texas A&M (Carter)	—	—	—	—	—	—	—	—	—	70T
U/Tulsa (Barker)	—	—	—	—	[illegible]	NFX	76	71	76	[illegible]
USGS (Hsei)	—	—	9	94	94T	—	—	—	—	—
U/Wisconsin (Wang)	—	—	—	—	—	57	38	—	—	40
Woods Hole (Hunt)	—	—	31	—	102	141	130	[illegible]	[illegible]	[illegible]
Woodward-Clyde, Pasadena (Burdick)	—	—	—	—	—	—	—	[illegible]	[illegible]	[illegible]
XDATA (Dines)	—	—	—	—	—	—	—	94	[illegible]	—
Yale U (Gordon)	—	—	—	—	46	4	38	26	39	104
Off-Site Totals	$472	$[illegible]	$[illegible]	$1,162	$1,[illegible]	$2,[illegible]	$3,[illegible]	$3,141	$4,[illegible]	$3,[illegible]

GEOSCIENCES RESEARCH (ERDA/DOE)
Historical Summary
(Operating Funds - Thousands)

ON-SITE	FY 1975	FY 1976	FY 1977	FY 1978	FY 1979	FY 1980	FY 1981	FY 1982	FY 1983	FY 1984
ANL	$ 98	$ 60	$ 50	$ 100	$ 140	$ 240	$ 310	$ 330	$ 330	$ 360
LANL	630	906	750	810	1,084	1,420	1,500	1,375	1,684	2,343
LBL	315	816	620	660	736	995	1,075	1,180	1,405	1,486
LLNL	75	136	130	250	630	910	1,060	1,110	1,280	1,815
ORNL	50	140	150	180	240	280	380	430	430	470
PNL	175	265	250	290	450	565	580	520	520	578
SNL/A	245	500	450	500	800	1,165	1,310	1,546	1,682	2,087
On-Site Totals	$1,588	$2,822	$2,400	$2,780	$4,079	$5,575	$ 6,215	$ 6,491	$ 7,331	$ 9,138
Total Off-Site	$ 672	$ 838	$ 899	$1,152	$1,895	$2,509	$ 3,030	$ 3,141	$ 4,523	$ 3,309
TOTAL OPERATING	$2,260	$3,660	$3,299	$3,932	$5,974	$8,084	$ 9,246	$ 9,632	$11,854	$12,447
TOTAL EQUIPMENT	—	—	—	—	$ 355	$ 560	$ 923	$ 900	$ 890	$ 960
TOTAL GEOSCIENCES	$2,260	$3,660	$3,299	$3,932	$6,329	$8,644	$10,168	$10,632	$12,744	$13,407

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Advanced Energy Projects FY 1984 Research Summaries

October 1984

U.S. Department of Energy
Division of Advanced Energy Projects
Office of Basic Energy Sciences
Office of Energy Research
Washington, D.C. 20545

OFFICE OF BASIC ENERGY SCIENCES

DIVISION OF ADVANCED ENERGY PROJECTS (AEP)

Program Description

What projects are supported?

This Division supports exploratory research on novel concepts related to energy. The research is usually aimed at establishing the scientific feasibility of a concept and, where appropriate, also at estimating its economic viability. Because projects supported inevitably involve a high degree of risk, an indication of a high potential payoff is required. An immediate, specific application of the concept is not an absolute prerequisite for consideration; thus, for example, proposers of schemes leading to the development of x-ray lasers are not required to justify their proposals by discussing potential applications of such lasers.

The concepts supported are typically at too early a stage of scientific verification to qualify for funding by DOE programs responsible for technology development. Where doubt exists, such programs are consulted, prior to proposal consideration by AEP, in order to establish their possible interest in the project.

Projects not supported

The AEP Division does not support ongoing, evolutionary research. Neither does it support large scale demonstration projects.

Period of support

By design the period of support is finite, generally not exceeding three years. It is expected that, following such a period, the concept will either be at a stage where it can be supported by a technologically appropriate organization or branch of DOE, or else it will be dropped.

Funding levels

The size of a contract in FY '84 varied between $48,000 and $390,000 per annum.

Who can propose?

Unsolicited proposals can be submitted by universities, industrial organizations, nonprofit research institutions or private individuals. Consideration is also given to ideas submitted by scientists working at national laboratories.

Proposal evaluation

Awards are based on the results of an evaluation process which usually involves a review by external reviewers. Regardless of the outcome of the evaluation, proposers receive copies of reviewers' reports.

Questions asked of the reviewers depend on the subject of the proposal. Some typical questions are listed below:

1. Is the proposed concept new? How does it compare with other work in the field?

2. Are there basic flaws in the scientific (technical) arguments underlying the concept?

3. Are the technological requirements of the proposed concept, including material requirements, within the realm of either present or near term future capabilities?

4. Is there anything about the concept which makes its economics manifestly untenable, even under reasonably optimistic assumptions?

5. Is the anticipated benefit to the public high enough to warrant the Government's involvement in the R&D effort?

Preproposals desired

It is suggested that before a formal proposal is prepared, the proposer should submit a brief outline of the proposed work. The outline should provide enough background information to enable a decision as to whether or not the proposed work programmatically fits the mission of AEP.

Proposals

Once a programmatic interest of AEP in the proposed project has been established, a proposal should be submitted along the guidelines specified in DOE/MA-0095, "Guide for the Submission of Unsolicited Proposals." Each proposal must contain:

- o A cover page, prepared in a format specified in DOE/MA-0095, Appendix B.

- A 200-300 word abstract, written in plain English, describing the essence of the project in terms understandable to a layman. The abstract should be in a form suitable for inclusion in DOE program presentations.

- A technical discussion of the proposed concept and a description of the proposed work. While the discussion should be kept brief, there is no formal limitation on the number of pages allotted to this section of the proposal. Since it is this section that will form the basis for the evaluations by technical reviewers, the proposer is urged to make certain that all aspects of the proposed project which are relevant to forming a judgment of the project's merits are adequately covered.

- A statement of work specifying all tasks to be performed in the course of the proposed work. A sample statement of work can be found on page 31.

- Description of available facilities.

- Resumes of key personnel.

- Detailed information on any support for the proposed or related work, past, present or anticipated, including proposals submitted, or about to be submitted, to other organizations.

- A cost estimate for the proposed effort.

Further Information

Inquiries should be addressed to:

Dr. Ryszard Gajewski, Director
Division of Advanced Energy Projects
Office of Basic Energy Sciences
ER-16, GTN
Department of Energy
Washington, D.C. 20545

Phone: 301/353-5995

OFFICE OF BASIC ENERGY SCIENCES

DIVISION OF ADVANCED ENERGY PROJECTS

Summaries of Projects Active in FY 1984

This section contains brief summaries of all projects active in this Division during Fiscal Year 1984 (October 1, 1983-September 30, 1984). The intent of this compilation is to provide a convenient means for quickly acquainting an interested reader with the program in Advanced Energy Projects. More detailed information on research activities in a particular project may be obtained by contacting directly the principal investigator shown below the project title. Some projects will have reached the end of their contract periods by the time this book appears, and will therefore no longer be active. Those cases in which work was completed in FY '84 are indicated by the footnote: *Project completed.

1. EXTREME ULTRAVIOLET AND SOFT X-RAY INSTRUMENTATION FOR MICROCHARACTERIZATION OF MATERIALS

Charles K. Rhodes

ALTEX CORPORATION
P.O. Box 10084
Chicago, Illinois 60610-0084

Date Started: August 15, 1984

Funding: FY '84 $250,000 for 12 months

Anticipated Duration: 2 years

High quality, short pulse, excimer laser systems are prime candidates for the generation of spectrally-bright coherent radiation in the extreme ultraviolet and soft x-ray spectral regions. Such excimer systems consist of (1) a unit generating a short, high-quality pulse at visible wavelengths, (2) a frequency shifter, and (3) a chain of ultraviolet amplifiers. Our objective is to develop a prototype laser system which delivers a tunable, high quality pulse of $\sim$ 10 psec duration in the range of <450 to 700 nm. In conjunction with suitable wavelength shifters, this instrument will cover the ultraviolet spectral range down to and probably below 240 nm. Its integration as the front end of an ultrahigh spectral brightness KrF laser system will result in a compact, low-cost laboratory instrument, delivering powers of > 10 GW at 5 eV photon energy. This new, powerful, and cost-effective technology would overcome the fundamental limitations of the low-brightness incoherent sources presently available and permit application to an unusually broad spectrum of important technical areas relevant both to pure scientific and industrial spheres.

2. THE CONTINUOUS MEMBRANE COLUMN: A LOW-ENERGY ALTERNATIVE TO DISTILLATION

BEND RESEARCH, INC.
64550 Research Road
Bend, Oregon 97701-8599

Walter C. Babcock
Membrane Separations Division

Date Started: February 5, 1982

Funding: FY '84 $134,000 for 12 months

Anticipated Duration: 3 years

The objective of this program is to evaluate membrane separation as an energy-efficient alternative to distillation. The study is focused on the separation of isopropanol from water, a process currently performed by distillation and azeotropic distillation. Work is under way in the areas of membrane development and assessment of membrane performance in a "continuous column" module configuration. Results thus far have been positive; for example, energy-consumption calculations based on membrane performance in laboratory tests indicate a 44% savings in energy is possible when a hybrid membrane/distillation approach is used in place of distillation alone to produce a 90 vol % isopropanol-in-water azeotrope.

3.* LIQUID MEMBRANES FOR THE PRODUCTION OF OXYGEN-ENRICHED AIR

BEND RESEARCH, INC.
64550 Research Road
Bend, Oregon 97701-8599

Harold K. Lonsdale
Membrane Separations Division

Date Started: April 16, 1979

Funding: FY '83 $302,000 for 12 months

Anticipated Duration: 5 years

The objective of this program is to develop novel liquid membranes for the energy-efficient concentration of oxygen from air. Oxygen-enriched air will find use in a wide range of industrial, chemical, and combustion processes. The liquid membrane consists of a solvent that contains a dissolved oxygen carrier and that is held within the pores of a membrane support. The oxygen carrier selectively transports oxygen across the liquid membrane by the process of "facilitated transport", which results in a product gas highly enriched in oxygen. Recent efforts have focused on increasing the flux of oxygen across these membranes by reducing their effective thickness. Work in progress relates to development of membrane modules in regeneration techniques to extend their life.

*Project completed

4. EXTREME ULTRAVIOLET COHERENT RADIATION DEVICE: TRANSVERSE OPTICAL KLYSTRON

BROOKHAVEN NATIONAL LABORATORY*
Upton, New York 11973

C. Pellegrini and A. van Steenbergen
National Synchrotron Light Source

Date Started: September 26, 1983

Funding: FY '84 $390,000

Anticipated Duration: 3 years

This project is for the development of a new radiation source to be incorporated with the VUV storage ring of the National Synchrotron Light Source (NSLS) which will produce coherent, radiation from 500 Å to 2000 Å. Specifically, this radiation source is a Transverse Optical Klystron (TOK) which makes use of a high power laser in the visible region and a permanent magnet undulator structure in conjunction with the circulating electron beam bunches in the storage ring to produce radiation at the harmonics of the laser. An exploratory experiment has been carried out with the installed FEL undulator. The design of an optimized, fixed gap, hybrid Vanadium Permendur - REC undulator is in progress, in addition to the design of the special vacuum chambers and overall optical configuration.

*Performed in cooperation with BELL LABORATORIES, 600 Mountain Avenue, Murray Hill, New Jersey 07974, Richard R. Freeman and Brian Kincaid co-principal investigators.

5.* FREE ELECTRON LASER TEST, NATIONAL SYNCHROTRON LIGHT SOURCE

BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

C. Pellegrini and A. van Steenbergen
National Synchrotron Light Source

Date Started: May 1, 1980

Funding: FY '83 $21,000

Anticipated Duration: 3 1/2 years

The purpose of this program is to develop a free electron laser test module driven by the circulating beam of a storage ring. The program will explore the effect of the free electron laser on the parameters of the storage ring as well as involve the development of a coherent wiggler to provide the appropriate mechanism for electromagnetic radiation amplification due to repeated interactions of the laser field and the transversely oscillating electrons in the undulator (coherent wiggler). It is anticipated that a basic design for a tunable high average power ultraviolet source with a narrow spectral bandwidth may result from these studies.

*Project completed

6.* MEQALAC CLUSTER
ION FUSION

BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

Lewis Friedman and Alfred Maschke
Chemistry & Accelerator Departments

Date Started: January 15, 1981

Funding: FY '82 $240,000 for 12 months

Anticipated Duration: 3 years

Proof-of-principle experiments are proposed to demonstrate that isotopic hydrogen molecule cluster ions can be prepared and accelerated. The long range goal of these experiments is the utilization of plasmas produced by accelerated cluster ions for the production of thermonuclear reactions. A cluster ion source has been developed which has produced low intensity beams of narrow mass distribution hydrogen clusters with mass to charge ratios as high as 10^4. Research on fundamental processes in this low temperature ion source designed to improve source intensity is in progress. A high precision "optical bench" beam transport system was developed for use with small aperture MEQALACs. High brightness beams of Argon and Xenon were accelerated in quadrupole focused acceleration columns. Laminar flow was observed in a 10 gap electrostatic quadrupole accelerating column and in a 50 quad transport line.

*Project completed

7. MOMENTUM RICH BEAM FUSION

BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

Alfred Maschke

Date Started: April 29, 1983

Funding: FY '84 $250,000 for 12 months

Anticipated Duration: 2 years

The objective of this study is to establish the feasibility of producing heavy ion beams with energies of a few hundred keV, and sufficient brightness that they might be used to implode a small volume of deuterium-tritium fuel. Computer simulations with the LASNEX code indicate that a beam temperature of around .1 eV, and an average current density of 10 mA/centimeter squared should be adequate to achieve thermonuclear ignition. A key element in achieving the high brightness is the laminar flow electrostatic quadrupole focused acceleration column that was developed under an earlier contract. Experimental results to date have measured the temperature of a Cesium beam from a hot tungsten contact ionization source. The beam temperature was found to correspond to the source temperature (about .1 eV). The acceleration column has been built and tested, and awaits being tested with beam.

8.* HIGH CURRENT BETATRON FOR A FREE ELECTRON LASER

UNIVERSITY OF CALIFORNIA
Irvine, California 92717

Norman Rostoker and Amnon Fisher
Department of Physics

Date Started: August 1, 1981

Funding: FY '81 $685,000 for 3 years

Anticipated Duration: 3 years

A modified Betatron is being developed that resembles an Astron. Electrons are injected into an elongated magnetic mirror. The Larmor radius is 6 cm; the distance between mirrors is 80 cm. With a field emission injector (50 kV, 1 amp, 150 nsec) about 20 nC have been trapped for about 10 μsec. The electron trajectories are helical with an axial period of 40 nsec and an azimuthal period of 3 nsec. Rapid data acquisition is facilitated by a 1 Hz repetition rate. The purpose of the experiment is to study injection, trapping, acceleration and extraction in this new configuration. Multiturn injection has been demonstrated with electrostatic and magnetic inflectors. Acceleration to about 1 MeV has been accomplished with an iron powder ferromagnetic core and increasing the field at the beam from about 100 to 1000 gauss while maintaining the Betatron 2:1 condition. Electrons have been extracted with a gate coil for direct measurement of the trapped charge. The injection is very nearly tangential to the cyclic orbit which should produce a high-current low-emittance beam suitable for a free electron laser. Measurements of the emittance of an extracted beam are the next objective.

*Project completed

9. ELECTROCHEMICAL AND ELECTROCATALYTIC PAIRED ORGANIC REACTIONS IN UNDIVIDED FLOW CELLS

UNIVERSITY OF CALIFORNIA
Los Angeles, California 90024

Ken Nobe
Department of Chemical Engineering

Date Started: July 1, 1984

Funding: FY '84 $70,000 for 12 months

Anticipated Duration: 3 years

Paired electrochemical syntheses for the production of organic chemicals can reduce energy consumption by as much as 50% compared to conventional electrochemical syntheses. A paired synthesis is more energy efficient because both the anodic and cathodic reactions contribute simultaneously to the formation of the final product(s). Additional energy savings can be achieved by performing the paired synthesis in an undivided flow cell and by incorporating an electrocatalytic hydrogenation as the cathodic partner of the paired reaction scheme. Moderate temperature, ambient pressure electrochemical hydrogenations at high surface area active electrocatalytic cathodes such as Raney nickel can be more energy efficient than chemical catalytic hydrogenations. The objectives of this research program are: 1) devise electro-organic paired syntheses, such as the oxidation and reduction of glucose to gluconic acid and sorbital, employing an active electrocatalytic cathode; 2) design, model and test continuous undivided flow cells for paired syntheses; and 3) evaluate the economic feasibility of the paired syntheses as opposed to producing the same chemicals individually by conventional chemical or electrochemical methods.

10. BIOEXTRACTION OF IRON FROM IRON OXIDES: REDUCTION OF COKE DEMAND IN STEEL PRODUCTION BY MICROBIAL BENEFICIATION

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California 91125

Michael R. Hoffmann
Engineering and Applied Science

Date Started: August 15, 1983

Funding: FY '83 $237,000 for 3 years

Anticipated Duration: 3 years

A research program is in progress to investigate the kinetics and mechanisms of the reductive dissolution of iron oxide minerals such as hematite, geothite, lepidocrocite, and magnetite as catalyzed by Thiobacillus thiooxidans, Pseudomonas sp.200, Bacillus acidocaldarius, Pseudomonas aeruginosa, and Bacillus circulans. Kinetic parameters are being obtained from batch and continuous flow reactor experiments in which the partial pressure of oxygen, temperature, pH, carbon source, and total reactive surface area are primary variables. Data obtained within the first year of work has shown clearly that Pseudomonas sp.200 is the most effective iron-reducing organism. Its characteristic maximum growth rate constant has been determined to be 0.4 hr^{-1}; this reaction rate constant indicates that P. sp.200 grows as fast as organisms active in biological reactors designed to treat domestic wastewater. The characteristic time for complete reductive dissolution of iron oxides and hydroxide solids is six to eight hours. Research is continuing on the mechanism of reductive dissolution. Plasmids of P. sp.200 have been isolated. They will be used to probe mechanistic details and to isolate and enhance the proteins responsible for iron reduction. Attempts will be made to isolate mutant strains of P. sp.200 capable of utilizing the Fe(II)/Fe(0) redox couple. If organisms possessing these capabilities are isolated and cultured continuously, it may be possible to produce elemental iron under ambient conditions.

11. NEW POLYMER ELECTRODES AND CONDUCTORS BASED ON POLY(HYDROQUINONE/QUINONE) OXIDATION/REDUCTION SYSTEMS

CASE WESTERN UNIVERSITY
Cleveland, Ohio 44106

Morton H. Litt
Department of Macromolecular Science

Date Started: September 15, 1983

Funding: FY '83 $277,000 for 14 months

Anticipated Duration: 14 months

This project has the following goals: 1) To synthesize soluble linear fused ring polyaromatic polymers (ladder polymers) which have attached 1,4-hydroxyl groups; 2) To characterize these polymers. The polymer should be a good electrical conductor. It is expected that the hydroxyl groups can be reversibly oxidized and reduced - making this material a good candidate for a very high capacity electrode. High molecular weight polymers will be made into oriented fibers and films and their mechanical properties as well as electrical properties studied. Fiber of these polymers should be like graphite fibers, but should be solution processable. Polymers have been made which have the proposed structure. At present, they are obtained in an insoluble form. Work is going on in two areas. First, the mechanism of polymerization is being studied. The objective here is to get soluble polymers. Secondly, the initial polymers are being oxidized, and their oxidation/reduction properties will be studied.

12.*DEVELOPMENT OF A BIOCHEMICAL
PROCESS FOR PRODUCTION OF
ALCOHOL FUEL FROM PEAT

Donald L. Wise

Funding: FY '83 $199,000 for 12 months

DYNATECH R/D COMPANY
99 Erie Street
Cambridge, Massachusetts 02139

Date Started: June 1, 1981

Anticipated Duration: 3 years

Peat and lignite represent a significant U.S. energy source. This research program is directed toward development of an aqueous, alkaline process for utilization of peat and lignite in liquid fuels production. The general approach to this process development can be described by three reaction chemistries. First, aqueous alkali is introduced to break the well-defined ethereal bonds in the peat and lignite structures and yield water-soluble carboxylic acids. Second, oxygen is added to promote the solubilization. Third, the solubilized aromatics are decarboxylated to give a water-immiscible aromatic fuel. An in-depth laboratory program has identified the necessary conditions for maximum breakdown of the peat and lignite to water-soluble carboxylic acids and for the greatest yield of decarboxylation products. Based on these results, preliminary conceptual designs and cost estimates were prepared for pilot and full-scale facilities.

*Project completed

13. CATALYSIS OF DIRECT METHANOL
ELECTRO-OXIDATION IN
BUFFERED ELECTROLYTES

S. Barry Brummer
Battery Division

Funding: FY '84 $146,000 for 12 months

EIC LABORATORIES, INC.
111 Downey Street
Norwood, Massachusetts 02062

Date Started: July 15, 1983

Anticipated Duration: 3 years

The objective of this program is the exploration of the catalysis of methanol oxidation in aqueous, concentrated $K_2CO_3/KHCO_3$ electrolytes for direct methanol/air fuel cells. A major goal of the program is the elimination of all noble metal catalysts. The $K_2CO_3/KHCO_3$ electrolyte has a suitable conductivity, however, its water vapor pressure is higher than desired at the operating condition of 100 to 200°C. It should be possible to reduce the water vapor pressure by addition of a co-electrolyte. The chemical and electrochemical stability of potential non-noble metal catalysts are being determined in the $K_2CO_3/KHCO_3$ electrolyte. The electro-oxidation of methanol is being examined with both stable non-noble and noble metal catalysts.

14.*INVESTIGATION OF THE EXTRACTION OF HYDROCARBONS FROM SHALE ORE USING SUPERCRITICAL CARBON DIOXIDE

James H. Porter

Funding: FY '82 $110,000 for 12 months

ENERGY & ENVIRONMENTAL ENGINEERING, INC.
1B Monsignor O'Brien Hwy
P.O. Box 215
E. Cambridge, Massachusetts 02141

Date Started: July 15, 1982

Anticipated Duration: 16 months**

Extraction of oil from shale was examined using carbon dioxide in its supercritical fluid state as the solvent. The experimental results showed that extraction yields were too low to be of commercial use at reduced temperatures ranging from 1.0 to 1.3 and at reduced pressures ranging from 1.0 to 2.8. Aqueous and hydrocarbon phases were extracted from the shale. The aqueous phase yield ranged from 1.6 to 4.0 times the hydrocarbon phase yield. Yields increased with increasing extraction time and as shale particle size was reduced. Yields also increased as the reduced temperature and solvent density increased. The hydrocarbon phase was predominantly alkanes and alkenes with boiling points ranging from 150 to 500°C.

*Project completed
**Includes unfunded extension

15. ULTRASONIC ATOMIZATION FOR COMBUSTION EFFICIENCY IN OIL BURNERS

William B. Tarpley, Jr.

Funding: FY '84 $117,000 for 12 months

ENERGY & MINERALS RESEARCH CO.
964 E. Swedesford Road
Exton, Pennsylvania 19341

Date Started: June 1, 1984

Anticipated Duration: 2 years

This project involves utilizing controlled oil feed to an ultrasonic area atomizer and involving an optimum combustion air interface. Investigation of novel methods of presenting the liquid to be atomized, novel methods of designing the ultrasonic visability face and mixing the low-velocity droplets with combustion air is to be carried out. Parametric relationships between liquid properties and ultrasonic variables will also be investigated.

16. DETECTION AND CHARACTERIZATION OF NOVEL METAL-BINDING PROTEINS

GENERAL ELECTRIC COMPANY
P.O. Box 8
Schenectady, New York 12301

David S. Holmes
Corporate Research & Development

Date Started: July 1, 1984

Funding: FY '84 $148,000 for 12 months

Anticipated Duration: 3 years

Metal binding proteins exist in nature. Apart from metalloenzymes, this unique group of organo-metallic molecules has received little attention. Yet metalloproteins might offer unique advantages for certain applications. These advantages include a remarkable specificity for binding individual metals or classes of related metals. This permits, for example, the chelation of silver in the presence of copper, or the chelation of virtually any transition or heavy metal in the presence of vast excesses of alkali metals such as sodium or potassium. More importantly, it is possible to isolate large quantities of metalloproteins and to modify them by using state-of-the-art genetic engineering. This latter ability could permit the construction of protein molecules exhibiting specificity toward more than one metal, with enhanced specificity towards one particular metal, or with enhanced functional stability. We propose to initiate a search for, and to characterize, novel metal-binding proteins in two unusual classes of microorganisms (Thiobacillus and Sulfolubus). These microorganisms exhibit unique advantages for this study including a remarkable tolerance to a broad range of metals in an acidic environment and the ability to oxidize many metals. Some of these organisms are thermophilic. Thermophilic proteins might exhibit enhanced functional stability or other unique properties.

17. FLUID DYNAMIC ENERGY SEPARATION

GEORGE WASHINGTON UNIVERSITY
Washington, D.C. 20052

J.V. Foa
School of Engineering and Applied Science

Date Started: September 15, 1983

Funding: FY '83 $294,000 for 2 years

Anticipated Duration: 2 years

The object of this study, the "energy separator", is a new kind of air conditioning and heating device that promises advantages of energy economy in a number of applications. This device has only one moving part, a free-spinning rotor, and its operating mechanism is very simple: it splits an initially uniform flow into two subflows and causes one of these to do work on the other. The energy separator derives its potential merit primarily from the fact that it permits the energy extracted from the cooling subflows to appear in the other subflow not as heat but rather in the form of recoverable mechanical energy. Experimental work has been in progress on three radically different models. An analysis has been developed for the selection of the configuration and operating conditions that will maximize the separation of energy under any given set of constraints, and its results are presently being used in the design of a fourth and improved experimental model. A study is also underway for the design of an air conditioning system that will incorporate this fourth model as its core component.

18.*RESEARCH AND DEVELOPMENT OF A MASS ACCELERATOR (MAID) AS A DRIVER FOR IMPACT FUSION

GT-DEVICES
5705A General Washington Drive
Alexandria, Virginia 22312

Derek Tidman and Shyke Goldstein

Date Started: May 6, 1981

Funding: FY '83 $297,000 for 12 months

Anticipated Duration: 3 years

The objective of this program is to demonstrate that high pressure plasma jets in the kilobar range can be used to propel solid projectiles to high velocity. The basic concept is to accelerate a solid mass (e.g., 0.5 gram) via a series of momentum kicks provided by sequentially directing the high pressure plasma jets onto the rear projectile surface as it passes through each module. This new approach to mass acceleration has been successfully demonstrated using 10 plasma discharge modules (with projectile sensing and timing circuits) aligned in a manner similar to a linear accelerator. Experiments in which the accelerator has been operated in a sense-and-kick mode have achieved velocities of 5.1 km/sec and a data base involving 575 shots has been established. The significance of this acceleration mechanism is that it can be used, in principle, to accelerate projectiles to several hundred kilometers per second as a driver for inertial fusion or another energy-related application. A theoretical base has also been developed to understand the physics of plasma jet generation and the coupling of the jet momentum to the projectile. This work has formed a solid basis for further experiments with larger scale devices.

*Project completed

19. MEASUREMENT OF THE EFFICIENCY OF MUON-CATALYZED FUSION

IDAHO NATIONAL ENGINEERING LABORATORY
EG&G Idaho, Inc., P.O. Box 1625
Idaho Falls, Idaho 83415

Steven E. Jones
Scientific Information AGM

Date Started: March 8, 1982

Funding: FY '84 $390,000 for 12 months

Anticipated Duration: 4 years

It is rather remarkable that the muon (symbol , an elementary particle like the electron) can induce the fusion reaction: $\mu + d + t \rightarrow \mu + He + n + 17.6$ MeV. We have observed eighty fusions caused by a single muon (on the average) in deuterium-tritium gases at room temperature. Thus, the muon serves as a catalyst for the fusion process, permitting it to proceed rapidly without the need for high (plasma) temperatures. Is muon-catalyzed fusion just a scientific curiosity or could power production be achieved? Results so far show that the reaction proceeds more rapidly then theoretically predicted. Morever, the loss of muons due to capture by the synthesized helium ion is significantly less than expected. Consequently, fusion energy yields are larger than anticipated - more than ten times the total energy of the muon driving the fusion reaction. Still, the output energy is less than the energy needed to initially produce a muon. Research continues in an effort to improve the energy balance.

20. GENERATION OF STIMULATED EMISSION IN THE SOFT X-RAY RANGE BY NONLINEAR PROCESSES WITH EXCIMER LASERS

UNIVERSITY OF ILLINOIS AT CHICAGO
Chicago, Illinois 60680

Charles K. Rhodes
Department of Physics

Date Started: September 15, 1983

Funding: FY '84 $52,000

Anticipated Duration: 2 years

High spectral brightness excimer lasers can be used to generate coherent extreme ultraviolet radiation by either harmonic generation or direct multiphoton excitation of appropriate laser media. Recent studies of two-photon pumped lasers in H_2 and HD at ~ 120 nm with conversion efficiencies of $\sim 10^{-2}$ and of a four-photon inner shell excited laser in Kr at 93 nm and with $\sim 10^{-4}$ efficiency, indicate that the latter mechanism, involving direct excitation, is considerably more promising. To study the basic properties of high order nonlinear processes in the ultraviolet, an experiment which evaluates the amount of optical energy transferred to various atomic species under collisionless conditions and at UV laser intensities of up to 10^{17} W/cm^2 is in progress. This experiment has led to the discovery of an anomalously strong energy coupling to high Z atoms which involves the absorption of as many as 99 photons. A time-of-flight photoelectron spectrometer which will address the question of state selectivity is in the testing phase. The experimental program is designed to (1) investigate the mechanisms leading to the anomalous ion production, (2) assess the limitations on the quantum state selectivity such processes can provide, and (3) attempt to observe genuine simulated emission in the 40 - 80 eV range. Success in this endeavor would imply the feasibility of a laboratory scale coherent source operating in the kilovolt range.

21. PRODUCTION OF ULTRAHIGH MAGNETIC FIELDS

JAYCOR
11011 Torreyana Road
San Diego, California 92138

Franklin S. Felber

Date Started: September 15, 1984

Funding: FY '84 $279,000 for 12 months

Anticipated Duration: 2 years

A general method has been discovered for producing controlled ultrahigh magnetic fields up to the order of 100 MG. The general method involves imploding a plasma in which a magnetic field has been entrained. The imploding plasma compresses the magentic field to high strengths. The optimal method for producing the imploding plasma appears to be a gas-puff Z pinch. The objective of this two-year experimental program is to produce and measure controlled utrahigh magnetic fields by this method. In the first year, the gas-puff Z pinch facility at the University of California at Irvine will be used for high-field tests at several megagauss. In the second year, a high-current gas-puff Z pinch facility will be used to demonstrate production of ultrahigh magnetic fields in the 15 to 20 MG range, which exceeds the highest controlled fields produced in this country. Applications for ultrahigh magnetic fields include reducing fusion ignition thresholds, producing collimated beams of gamma radiation, accelerating particles, and producing high-energy densities (hundreds of eV/A^3) under controlled conditions for studies of plasma physics, atomic physics, and material properties.

22. FREE ELECTRON LASER AT THE ETA*

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

A.M. Sessler and D. Prosnitz

Date Started: February 8, 1982

Funding: FY '83 $360,000 for 12 months

Anticipated Duration: 38 months

The purpose of this experiment is to develop a tapered-wiggler Free Electron Laser (FEL) as an efficient microwave source between 35 and 40 GHz. An application of this source is as electron cyclotron resonance heating of thermonuclear plasmas and a second application is as a high peak power source for high energy particle acceleration. The Lawrence Livermore National Laboratory's Experimental Test Accelerator provides the high-current, high voltage (1 kA, 4 MeV) low emittance electron beam used to drive the FEL amplifier. The electron beam wiggler which is electromagnetic, has no iron, and is pulsed; there is microwave input and microwave output diagnostics. Initial operation was developed a 8 mm wavelength, with the capability of studying 2 mm and 4 mm in the future. Beams of up to 450 A have been transported through the wiggler and super-radiant oscillations from noise have been observed as a function of length. This radiation (about 1 kW), which is coherent, has a gain of 13 dB/m and shows no sign of saturation in the 3 m wiggler. In an amplifier mode, with 23 kW fed in from a magnetron, the untapered wiggler, when tuned to resonance, gives 80 MW. Further study of the physics of a tapered FEL is planned.

*Experimental Test Accelerator at Lawrence Livermore National Laboratory.

23.*DETECTION AND ENRICHMENT OF FRACTIONALLY CHARGED PARTICLES IN MATTER

LAWRENCE LIVERMORE NATIONAL LABORATORY
P.O. Box 808, L-482
Livermore, California 94550

Charles D. Hendricks
Y Division, Laser Program

Date Started: May 1, 1982

Funding: FY '84 $290,000 for 12 months

Anticipated Duration: 3 1/2 years

This project is an experimental search for fractional charged particles in matter. Such particles may be a manifestation of free quarks. At the heart of the experiment is a charge-to-mass measurement on very uniform mass particles. Thus, a measurement of q/m will yield relative values of the charge of the particles. Because most of the particles should have charges which differ by integer values of one electron charge, only relative charge measurements between particles need be made to determine the presence of fractional charges. Liquid drops which are about 45 micrometers diameter and spaced about 750 micrometers apart are made at a rate of approximately 3×10^4 drops per second. These values depend on the particular parameters set into the experiment as it is being done. The drops traverse the space between two vertical, parallel plates which may be maintained at a DC potential difference up to about 60 kV. With no potential between the plates the drops travel along a straight vertical line downward between the plates. With a high potential between the plates, the drops are deflected transversely along paths which depend on the charge on each drop. Data is being taken to determine the realtive charges on the drops and, thus, determine the presence or absence of fractional charges.

*Projects 23 and 28 are cooperative interlaboratory projects.

24. PUMPING OF GAMMA-RAY LASERS: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS

LOS ALAMOS NATIONAL LABORATORY
Los Alamos, New Mexico 87545

G. C. Baldwin
Physics Division

Date Started: September 27, 1983

Funding: FY '84 $290,000 for 12 months

Anticipated Duration: 3 years

This project comprises a set of investigations related to concepts for exciting a laser that could operate with recoilless nuclear transitions in the sub-nanometer region without requiring excessive pumping power. Experiments to develop a technique for preparing a nuclear population inversion by selective photoionization of atoms containing the nuclear isomer Hg-197 are nearing completion. Another experiment in preparation is intended to demonstrate an effect of atomic (optical) excitation on the decay rate of the low-lying isomer of U-235. Theoretical investigations are addressing the problems of 1) transferring populations from long-lived isomers to short-lived nuclear states that can emit recoilless gamma radiation; 2) identifying nuclides with appropriate properties; 3) Mossbauer superradiance, which should govern the kinetics of the resultant gamma-ray emission.

25. MAGNETIC REFRIGERATION FOR EFFICIENT CRYOGEN LIQUEFACTION

LOS ALAMOS NATIONAL LABORATORY
P.O. Box 1663, KS M764
Los Alamos, New Mexico 87545

John A. Barclay
Group P-10

Date Started: February 1, 1982

Funding: FY '84 $270,000 for 12 months

Anticipated Duration: 3 1/2 years

The objective of this work is to consider conceptual designs, test models of those designs, and develop a data base for compact, reliable, high-efficiency magnetic refrigeration, with special emphasis on application of this technology to liquefaction of cryogens. Data base generation consists of literature evaluation and experimental work. Files on magnetic materials, fluid dynamics, heat transfer, pumps, drive motors, dewars and magnets are being compiled. Experimental results on the physical, thermomagentic, transport, and mechanical properties of several intermetallic rare earth compounds have shown that several materials may be suitable magnetic refrigerants between 4 K and 300 K. Examples include GdNi, GdPd, GdRh, GdZn and $ErAl_2$. Characterization of these materials continues. Heat transfer in magnetic refrigerators has been carefully studied including optimization of several geometries. Effective regeneration has been identified as a key problem for high-efficiency designs. Pump and drive motor efficiencies have been measured and are an area of concern. Using the data base information, a one watt 4 - 20 K refrigerator model has been designed, built and is entering the test mode. Several key problems in this temperature range have been identified and are being investigated. Design work on a 20 - 77 K device is underway.

26. THEORETICAL STUDY OF MUON-CATALYZED FUSION

LOS ALAMOS NATIONAL LABORATORY
P.O. Box 1663
Los Alamos, New Mexico 87545

James S. Cohen
Theoretical Division

Date Started: December 29, 1983

Funding: FY '84 $202,000 for 12 months

Anticipated Duration: 3 years

By virtue of the muon (μ^-) being about 200 times as massive as the electron, the molecular ion $(dt\mu^-)^+$ is small compared to ordinary DT^+ and nuclear fusion occurs rapidly in it. The muon is usually freed after fusion and available to catalyze more reactions. In recent experiments on muon-catalyzed fusion in dueterium-tritium mixtures at high densities, almost 100 fusions per muon have been observed. However, enough information is not yet available to evaluate potential applications of muon catalysis. It is still desirable to explore new ideas for enhancing muon utilization. The present theoretical effort is designed to provide understanding of the observed kinetics and suggest improvements. There remain several foundamental processes which require further investigation, and theory is essential in this task. Problems being researched include muon production, muon capture by molecules, effects of impurities, resonant muonic molecule formation, muonic molecule binding energies and wave functions, muon sticking to the fusion alpha particle, and possibilities of reactivation if sticking occurs.

27. LIQUID METAL THERMO-ACOUSTIC ENGINE

LOS ALAMOS NATIONAL LABORATORY
Los Alamos, New Mexico 87545

J. C. Wheatley
Physics Division

Date Started: September 27, 1983

Funding: FY '84 $370,000 for 12 months

Anticipated Duration: 3 years

This project is concerned with studying a new type of thermoacoustic heat engine using a liquid metal, such as liquid sodium, as the working substance. The thermophysical properties of liquid sodium make it far superior to ideal gases as working substance in such an engine because of its very low Prandtl number, high density, and high sound velocity. We have developed an accurate theory of the thermoacoustics of liquid metals in acoustic engines, and, with a computer code based on it, studied optimization of the acoustic design of prime movers. In order to convert the acoustical power output to electricity, a more useful form of energy, we studied theoretically two approaches: an a.c. magnetohydrodynamic generator, in which the high electrical conductivity of sodium is used, and a variable reluctance generator. Both schemes are characterized by extreme mechanical simplicity. We have designed and are now constructing a laboratory engine to test the theory of the thermoacoustics, the magnetohydrodynamic generator, and the variable reluctance generator. The test engine is designed to produce 600 W of acoustic power at 31% of Carnot efficiency in a 4 cm diameter engine operating between 1000 K and 400 K.

28.*DETECTION AND ENRICHMENT OF FRACTIONALLY CHARGED PARTICLES IN MATTER

LOS ALAMOS NATIONAL LABORATORY
P.O. Box 1663
Los Alamos, New Mexico 87545

George Zweig
Theoretical Division

Date Started: May 1, 1982

Funding: FY '84 $334,000 for 12 months

Anticipated Duration: 3 1/2 years

The basic unit of electric charge is one third that of the electron. It is therefore natural to ask if isolated particles of fractional charges ± 1/3e, ± 2/3e, ± 4/3e. . . . exist freely as elements of the earth. William Fairbanks' group at Stanford University has concluded that they do. Negative fractionally charged particles are interesting because they could replace electrons in atoms, molecules and solids, leading to super-dense states of matter. Under certain circumstances they would even catalyze fusion reactions. This project is a combined theoretical and experimental effort to search for fractionally charged particles in a wide variety of materials, to determine which materials are most abundant in fractionally charged particles, and to enrich the fractional charge content of sample materials. The crystal chemistry of fractionally charged particles is being theoretically developed and those materials most likely to contain enhanced concentrations of fractionally charged atoms are being identified. These materials will then be obtained, analyzed and used as samples for the experimental studies.

*Projects 23 and 28 are cooperative interlaboratory projects.

29. RESEARCH ON MILLIMETER AND SUBMILLIMETER RADIATION FROM ROTATING ELECTRON BEAMS IN RIPPLED MAGNETIC FIELDS

UNIVERSITY OF MARYLAND
College Park, Maryland 20742
MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts 02139

William W. Destler, Univ of MD
George Bekefi, MIT

Date Started: July 1, 1984

Funding: FY '84 $146,000 for 12 months

Anticipated Duration: 2 years

The production of millimeter and submillimeter radiation from rotating electron beams interacting with an azimuthally periodic wiggler magnetic field is being studied experimentally and theoretically. Initial studies using a 2 MeV, 1 kA, 6 cm radius rotating beam interacting with a 1400 gauss wiggler field with six spatial periods around the azimuth have produced in excess of 200 kW of power in the frequency range 90-170 GHz. The radiation frequency spectrum is being measured in this range using a grating spectrometer, and the effects on radiation production of variations in electron energy, current, pulse length, and wiggler periodicity and magnitude are currently being investigated. A long pulse (5 μs), low voltage (40 kV) experiment is currently in the design stages.

30. MAGNETIC ENHANCEMENT AND
DEMINERALIZATION OF EASTERN
COALS

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts 02139

David R. Kelland
Francis Bitter National Magnet Lab

Date Started: June 1, 1984

Funding: FY '84 $389,000 for 12 months

Anticipated Duration: 3 years

The inorganic sulfur and mineral content of high sulfur coals can be reduced by high gradient magnetic separation (HGMS). Enhancement of the magnetization of the mineral pyrite through selective heating by microwave irradiation to convert pyrite to more magnetic pyrrhotite should improve demineralization performance. This research program, to be carried out in cooperation with General Electric-Schenectady, will attempt to verify indications of successful microwave pretreatment of coals and investigate the effect of magnetic enhancement on HGMS performance on coals with insufficient pyrrhotite for effective magnetic desulfurization. Success in using HGMS on direct desulfurization on some coals and on converted pyrrhotite in coal liquids is an indication that improved magnetic enhancement by the recently observed effect of localized surface discharges should dramatically affect HGMS demineralization. The concept of effective selective heating and of combining magnetic enhancement with mineral separation needs to be proved feasible. A study of the conversion mechanism and necessary residence time will provide data for extending an encouraging early economic and engineering analysis of this method of precombustion coal cleaning.

31.*ZONE-MELTING RECRYSTALLIZATION
FOR SOLAR CELLS

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
77 Massachusetts Avenue
Cambridge, Massachusetts 02139

Henry I. Smith
Electrical Engineering & Computer Science

Date Started: September 1, 1982

Funding: FY '84 $20,000

Anticipated Duration: 2 years

The objective of this project is to develop a process for producing oriented silicon films suitable for low-cost solar cells. A new technique, zone-melting recrystallization (ZMR), has been developed which produces crystalline silicon films having mobilities close to bulk values. Using a vertical-constriction technique, (100) texture has been obtained in films 60 μm thick. Single-grain films are produced by passing the molten zone through a lithographically-defined planar constriction. Solar cells have been fabricated using ZMR in conventional homojunction and interdigitated contact form. Current-voltage traces show a departure from ideal diode behavior principally due to shunt resistance effects. Efforts to isolate fabrication-induced defects are underway in which contact resistances and alloying procedures will be studied. Spectral response measurements indicate that cells produced by ZMR have current collection efficiencies comparable to cells fabricated in Czochralski silicon, and a minority carrier diffusion length of 30-100 μm in an unpassivated Si film. This has been confirmed by electron beam-induced current (EBIC) and diode reverse recovery techniques.

*Project completed

32.*DEVELOPMENT OF DIRECT-CONTACT, HIGH EFFECTIVENESS DROPLET HEAT EXCHANGERS

MATHEMATICAL SCIENCES NORTHWEST, INC.
2755 Northup Way
Bellevue, Washington 98004

William J. Thayer III
Flow Technology Group

Date Started: July 1, 1981

Funding: FY '83 $257,000 for 12 months

Anticipated Duration: 3 years

A reliable technique for transferring heat between gas and liquid streams in the 1200-2000 K temperature range could greatly improve the efficiency of industrial processes and power generation systems. The objective of this program has been to evaluate direct contact heat transfer between counterflowing droplets and gas as a means of eliminating the limitations of conventional heat exchangers imposed by solid walls. Computer codes have been developed to evaluate multi-dimensional, two-phase flow and heat tansfer aspects and losses of droplet heat exchangers. Tests have been conducted to characterize, evaluate, and demonstrate processes which control the flow and heat transfer processes between counterflowing droplets and gas, and the formation of uniform droplets of viscous, high-surface-tension materials that simulate molten salts and slags. Comparisons of test data and model predictions have confirmed projected trends and demonstrated higher effectiveness heat transfer than expected. Cycle analyses and applications studies indicat [illegible] at the droplet heat exchanger could provide energy savings of 70 percent by making p [illegible] igh temperature waste heat recovery from dirty, corrosive gas streams. .

*Project completed

33. PERVAPORATION: A LOW-ENERGY ALTERNATIVE TO DISTILLATION

MEMBRANE TECHNOLOGY AND RESEARCH, INC.
1030 Hamilton Court
Menlo Park, California 94025

Richard Baker

Date Started: April 15, 1983

Funding: FY '84 $89,000 for 8 months

Anticipated Duration: 20 months

The object of this project is to develop selective pervaporation membranes. Pervaporation is a membrane separation process that could offer substantial energy savings compared to distillation. The principal problem inhibiting the development of pervaporation is the lack of suitably selective membranes. Thin film composite membranes have been made and evaluated in laboratory membrane cells and as small modules. Based on the experience obtained with these model mixtures we are determining the applicability of pervaporation to more economically significant organic mixtures. This data will be used to perform a technical and economic analysis of the process.

34.* EXPERIMENTAL RESEARCH IN HIGH TEMPERATURE SOLAR THERMOCHEMICAL PROCESSING. HYDROGEN AND SULFUR FROM HYDROGEN SULFIDE

UNIVERSITY OF MINNESOTA
111 Church Street, S.E.
Minneapolis, Minnesota 55455

Edward A. Fletcher
Department of Mechanical Engineering

Date Started: July 16, 1982

Funding: FY '82 $229,000 for 24 months

Anticipated Duration: 2 years

Highly concentrated sunlight is uniquely suited for supplying process heat at very high temperatures. The efficiency with which process heat is used to effect endothermic processes increases as the temperature at which the heat is added increases. This project makes use of a highly-concentrating solar furnace to study the production of hydrogen and sulfur from hydrogen sulfide in a high-temperature thermochemical process. We have studied the effect of hydrogen sulfide and its decomposition and oxidation products, as well as admixed hydrocarbons, on material for reactor construction, constructed three reactor-separators and their appurtenances, have evaluated various techniques for the construction of effusion membranes, and are now conducting experiments to test the efficacy of the process and evaluate the cost benefits which may be achievable by these kinds of processes vis-a-vis conventional methods of handling hydrogen sulfide.

*Project completed

35.* HOLOGRAPHIC TECHNOLOGY FOR SOLAR ENERGY CONCENTRATION

NATIONAL TECHNICAL SYSTEMS
12511 Beatrice Street
Los Angeles, California 90066

Tomasz Jannson
Research Division

Date Started: June 1, 1981

Funding: FY '83 $204,000 for 12 months

Anticipated Duration: 3 years

The objective of this project is to explore the possibility of using dichromated-gelatin holographic technology for solar energy concentration. Special emphasis has been given to spectrum-splitting holoconcentrators. During Fiscal Year 1984, significant progress has been made in the photochemistry, physics and optics of the holoconcentrators. It was verified that in Lippmann geometry, the reflectivity of the selective holographic mirrors can reach at least 99.9%, i.e. the photochemistry of the dichromated gelatin to a very good approximation preserves the physical properties of reflection Bragg holograms (predicted by Kogelnik theory and by the more general non-uniform WKB theory). In holoconcentrator geometry, the hologram diffraction efficiency, limited only by Fresnel losses has been obtained (up to 92%) and it was shown that in the case of zero-dispersion gratings with curved holographic coatings, the optical efficiency of the holoconcentrator system can reach this value. Hence, the holoconcentrator systems can be uniquely very close to the ideal PV spectrum-splitting systems. Moreover, several additional attractive holographic applications, such as high efficiency selective reflective filters, holo-windows and laser-protection selective mirrors, have been developed. The next generation of holoconcentrators will integrate focusing and spectrum-splitting of the visible spectrum, in the reflection mode, and focusing of near IR spectrum, in the transmission mode.

*Project completed

36. HIGH-FLUX, EXTENDED-PULSE ION ACCELERATOR

UNIVERSITY OF NEW MEXICO
Albuquerque, New Mexico 87131

S. Humphries, Jr.
Department of Chemical and Nuclear Engineering

Funding: FY '83 $267,000 for 3 years

Date Started: September 27, 1983

Anticipated Duration: 3 years

The objective of this program is to develop novel accelerator technology for ion implantation and materials modification. The technology is based on neutralization of ion beams by low energy electrons and control of the electrons through transverse magnetic fields. Plasma sources and acceleration gaps under investigation are capable of current density above 1 A/cm2 for pulselengths from 0.1 to 1 ms. A vacuum arc array has produced 25 A pulses of Al^+ ions; the geometry is suitable for a wide variety of metal ions. A second generation cross-field discharge source is currently being tested for ionization of gaseous species. The second year of the program will concentrate on studies of post-acceleration in a single gap. A 20 kV electrostatic test stand has been constructed for this purpose.

37.* MODIFICATION OF THE SURFACE TEMPERATURE BY AN ARTIFICIAL CIRRUS CLOUD

STATE UNIVERSITY OF NEW YORK
Albany, New York 12222

Bernard Vonnegut and Peter Chylek
Atmospheric Sciences Research Center

Funding: FY '80 $244,000 for 36 months

Date Started: September 1, 1980

Anticipated Duration: 3 1/3 years**

The objective of this project was to explore the practicality of using artificially formed cirrus clouds to achieve significant energy savings in densely populated areas. Meteorological data for about 10 years in the Albany area have been analyzed to determine how often the situation favorable for formation of an artificial cirrus cloud occurs. Preliminary results indicate that a suitable situation in the middle and upper troposphere occurs about 10 times per cold season. The combined effect of clearing clouds during the daytime and making cirrus clouds during nighttime gives a benefit-to-cost ratio of about 4/1 for the Albany area. For large metropolitan areas the benefit-to-cost ratio may be up to 40/1. Experimental work carried out at the University of Alaska's site at Fairbanks was concerned with observing the details of how light is scattered by clouds of water droplets and ice crystals. Analysis has also been carried out on about 10 years of data showing the effect of cirrus clouds over Mauna Loa on hourly average diffuse and direct solar radiation. This analysis can be used to suggest what effects artificial cirrus clouds would have on solar radiation reaching the surface. A radiative-convective climate model has been used to estimate the effect of increased cloudiness on the surface temperature, and radiative properties of ice clouds have been studied.

*Project completed
**Includes unfunded extension

38. VALIDATING THE PARAMAGNETIC LOGGING EFFECT

PARAMAGNETIC LOGGING, INC.
3123 - 198th Place S.E.
Bothell, Washington 98012

W. Banning Vail

Date Started: August 1, 1984

Funding: FY '84 $109,000

Anticipated Duration: 15 months

The Paramagnetic Logging Effect (PLE) is a recently predicted new magnetic phenomenon which will serve as the physical basis of a new borehole device capable of the direct measurement of the volume of petroleum reserves around a cased drill-hole to a radius of 50 feet or more into formation. The nucleons chemically bound in water and oil present in formation are preferentially aligned in the earth's magnetic field causing the natural nuclear paramagnetism within the formation. This paramagnetism causes a slight alteration in the strength of the earth's magnetic field in the vicinity of a borehole adjacent to the formation. Repeated application of an A.C. magnetic field at the Larmor frequency of the nucleons present yields an amplitude modulation of the earth's magnetic field. The magnitude of such modulation yields the total number of nucleons present and the phase contains information used to separate oil and water and identify the viscosity of oil present. The purpose of the project is to systematically study the new physical effect in a 4,800 gallon plastic tank which will be filled with water, then oil, and finally with mixtures of oil and water. The influence of borehole casing on these results will also be studied.

39.* ENERGY SYSTEMS BASED ON POLYACETYLENE: RECHARGEABLE STORAGE BATTERIES AND SCHOTTKY BARRIER SOLAR CELLS

UNIVERSITY OF PENNSYLVANIA
3451 Walnut Street
Philadelphia, Pennsylvania 19104

A. G. MacDiarmid
Department of Chemistry

Date Started: March 1, 1981

Funding: FY '82 $101,000

Anticipated Duration: 3 years

Research has continued on the evaluation of polyacetylene, $(CH)_x$, the prototype conducting polymer as an electrode-active material in novel rechargeable batteries. There are currently only two, widely used rechargeable batteries -- the lead/acid battery and the nickel/cadmium battery. In view of the adverse environmental effects of cadmium it is essential to evaluate other types of cells as a possible replacement for the Ni/Cd battery, in the event this should become necessary. Conducting polymers offer a potentially enormous new type of non-toxic material for use in rechargeable batteries. The $TiS_2/Li^+A^-/Li$ cell (A^- = anion) which exhibits many excellent properties, suffers from a major disadvantage caused by the formation of Li dendrites on continued charging and discharging. We have developed a battery of the form $TiS_2/M^+A^-/[M^+y(CH)^{-y}]_x$ where M = Li^+ or Na^+ and A^- = $(ClO_4)^-$ or $(PF_6)^-$ in which this problem has been elminated by replacing the Li with n-doped polyacetylene. This cell exhibits excellent recyclability, coulomb efficiency and retention of charge. Preliminary studies of "polyaniline", which is stable in air and water, show that it might also serve as an excellent electrode-active material.

*Project completed

40.*IMPLODING PLASMA X-RAY LASER

PHYSICS INTERNATIONAL
2700 Merced Street
San Leandro, CA 94577

Sik-Lam Wong

Date Started: September 1, 1981

Funding: FY '83 $375,000 for 12 months

Anticipated Duration: 2 1/2 years

A collisionally pumped Ne-like krypton x-ray laser scheme is being investigated using an imploded plasma source ($\sim$4 cm x 0.5 mm). The implosion is driven by the 5 TW Defense Nuclear Agency PITHON electrical pulse generator. According to theories developed at Lawrence Livermore National Laboratory, the measured plasma temperature ($T_e \sim 1$ keV) and density ($N_e \sim 10^{21}$ electrons/cm^3) are nearly ideal for producing population inversions in XUV ($\sim$83-100 eV) 3-3 Ne-like krypton transitions. Time integrated XUV spectral data are consistent with population inversion for 8 transitions. The measured line widths are about five times broader than that expected from doppler broadening and may be due to non-thermal plasma conditions. As a result, the gain in the lasing medium is about 0.5/cm. The available plasma length is 3.5 cm over a 2 ns time frame. We are investigating a number of schemes to reduce the linewidths, and thus increase the gain, by changing the plasma conditions, e.g., imploding a gas puff on an axial krypton plasma and use of an axial B-field for stabilizing the plasma.

*Project completed

41.*SOFT X-RAY LASING ACTION IN A CONFINED PLASMA COLUMN

PRINCETON UNIVERSITY
Princeton, New Jersey 08544

Szymon Suckewer
Plasma Physics Laboratory

Date Started: September 13, 1979

Funding: FY '83 $329,000 for 12 months

Anticipated Duration: 4 years

The objective of this project is an experimental investigation of lasing action in the soft x-ray spectrum region at wavelengths 182 Å, 135 Å and 520 Å corresponding to the 3→2, 4→2, and 4→3 transitions in the CVI ion. The basic idea is to use a multi-Z (e.g., carbon, oxygen) thin plasma column confined by a strong longitudinal magnetic field (100 kG), first heated by a CO_2 laser and then cooled rapidly by radiation losses. Calculations indicate a total gain in excess of 100 for the 3→2 transition, in excess of 10 for the 4→2 transition, and in excess of 300 for the 4→3 transition for a 10 cm long plasma column heated by a 10-20 GW CO_2 laser beam. Experiments showed good plasma confinement in magnetic fields 50-100 kG and effective radiation cooling of such a plasma, especially with additional small amounts of higher-Z elements such as Ar or Xe. Measurements of gain for CVI 4→3 (520 Å) and 3→2 (182 Å) transitions indicate the possibility of obtaining a high gain for 4→3 transitions, and also for the 3→2 transitions with improved CO_2 laser optics.

*Project completed

42. DEPOSITION OF HIGH QUALITY CuInSe$_2$ BY SPRAY PYROLYSIS

RADIATION MONITORING DEVICES, INC.
44 Hunt Street
Watertown, Massachusetts 02172

Gerald Entine

Date Started: September 15, 1982

Funding: FY '83 $116,000 for 12 months

Anticipated Duration: 2 3/4 years

The ultimate success of any terrestrial photovoltaic energy conversion approach requires that the following factors be satisfied: 1) high individual solar cell conversion efficiency, 2) low cost per unit area to produce the cells, 3) adequate availability of the constituent materials to produce the cells, 4) long term stability. CuInSe$_2$ is a material which promises to meet these requirements, but to date can only be made using expensive laboratory techniques. This project is a proof-of-concept effort to show that CuInSe$_2$ can be prepared by spray pyrolysis. CuInSe$_2$ is a promising solar cell material and spray pyrolysis is a technique well-suited for use in a manufacturing process. High quality, uniform and continuous films have been produced and solar cell device testing is underway.

43. IONIZATION FRONT ACCELERATOR

SANDIA NATIONAL LABORATORIES
Albuquerque, New Mexico 87185

Craig L. Olson
Plasma Theory Division - 1241

Date Started: June 1, 1981

Funding: FY '84 $190,000 for 12 months

Anticipated Duration: 3 1/2 years

The goal of this project is to accelerate ions to high energies using the large space charge field (~100 MV/m) from the potential well at the head of an intense relativistic electron beam (IREB). The Ionization Front Accelerator (IFA) uses laser photoionization of a special working gas to control the motion of the potential well. A second generation system (IFA-2) is now operational. This system includes an IREB machine (1.0 MV, 30 kA, 30 nsec) with laser-triggered switches with a command firing jitter of 1 nsec, a beam conditioning cell to steepen the current rise time to < 3 nsec, a heated experimental cell with Cs as the working gas, a dye laser (852.1 nm) to pre-excite the Cs, an XeCl laser (308 nm) to photoionize the excited Cs, a Pockels deflector to provide a continuous sweep of the XeCl laser beam, and beam front and ion diagnostics. The deflector system produces a quadratic temporal sweep of the XeCl laser beam over 30 cm in 20 nsec, but it has a transmission efficiency of only ~3% and delivers $\lesssim$0.15 mJ/cm^2 in the swept beam. Initial tests with the "lasers early" demonstrate that the photoionization scheme works, and that an XeCl laser intensity of $\gtrsim$ 0.5 mJ/cm^2 is required to control the front, in agreement with theoretical calculations. Intense efforts are being made to increase the swept XeCl laser beam intensity to the required level for successful IFA operation.

44.*PLANAR FLOW CASTING OF SHEET SILICON FOR PHOTOVOLTAIC CELLS

SOURCE TECHNOLOGY APPLIED METALLURGICALS, INC.
SOLAMAT DIVISION
885 Waterman Avenue
East Providence, Rhode Island 02914

Mandayam C. Narasimhan

Date Started: August 1, 1982

Funding: FY '83 $208,000 for 12 months

Anticipated Duration: 2 years

The object of this research program is to evaluate the castability of silicon sheets for photovoltaic application by the planar flow casting process and a newly developed roller quench casting process. The double roller quench casting process was used to cast sheet silicon 100 to 625 microns thick, 2 to 7 cm wide and 15 to 40 cm long at casting speeds of 10 to 90 meters per minute. This process works both in ambient and inert atmosphere. These sheets consists of columnar grains having in plane dimensions between 100 to 1000 microns. Sheets which are p-type with electrical resistivities in the 5 to 20 ohm-cm range have been prepared and solar cells have been fabricated. A solar conversion efficiency of 8.7% has been demonstrated under air mass-1 solar spectrum with a non-optimized anti reflection coating on the solar cells. Methods to improve the casting process reliability and techniques to improve solar cell efficiency are under investigation.

*Project completed

45. SYNTHESIS AND PHOTOELECTROCHEMICAL CHARACTERIZATION OF SEMICONDUCTING GROUP VIII TRANSITION METAL CHALCOGENIDES AND PNICTIDES

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

Bruce Parkinson
Photoconversion Research Branch

Date Started: September 26, 1983

Funding: FY '84 $172,000 for 12 months

Anticipated Duration: 2 years

Semiconducting electrodes, which are illuminated in the proper solution, are capable of converting solar energy directly into useful chemicals and fuels. Conventional semiconductor materials do not contain the elements (Fe, Co, Ni, Ru, Rh, Pd, Os, Ir, Pt) which are known to be most active for the catalytic conversion of simple molecules (CO_2, H_2O, CO, N_2) to useful fuels and chemicals (HCO_2H, H_2, O_2, CH_3OH, NH_3, N_2H_2, CH_2O). We have been synthesizing and growing crystals of new semiconductors (i.e., PdPS, PdPSe, PdP_2, $Pd_3(PS_4)_2$, PtS_2), containing group VIII metals combined with a chalcogen (S, Se, Te) and/or pnicogen (P,As), and examining their electronic properties (bandgap, carrier type and mobilities, doping densities etc.) with photoelectrochemical techniques. Materials with suitable electronic properties and stability to photocorrosion reactions will be tested for catalytic activity towards the reactions of interest.

46. GAS-LOADED, FREE-ELECTRON LASER

STANFORD UNIVERSITY
Stanford, California 94305

Richard H. Pantell
School of Engineering

Date Started: August 1, 1984

Funding: FY '84 $381,000 for 12 months

Anticipated Duration: 3 years

The objective of this program is the demonstration of a high peak power, coherent source tunable over the range from 5000 Å to 2000 Å. An innovative feature is the introduction of a gas into the interaction region of an FEL so as to provide a refractive index for phase matching the optical wave to the relativistic electron beam. The additional degrees of freedom made available in the choice of wiggler parameters and electron beam energy lead to much higher gains and less costly components than is possible in the vacuum FEL for these wavelengths. Theoretical considerations of electron scattering and ionization of the medium have led to the choice of hydrogen for the gas and to an electron beam energy of 40 MeV. Gains of order 20% per pass are predicted for this design at gas pressures of a few atmospheres.

47. COGENERATION OF ELECTRIC ENERGY AND USEFUL CHEMICALS IN A HIGH TEMPERATURE FUEL CELL

TUFTS UNIVERSITY
Medford, Massachusetts 02155

Michael Stoukides
Department of Chemical Engineering

Date Started: April 1, 1984

Funding: FY '84 $90,000 for 12 months

Anticipated Duration: 2 years

Solid electrolyte fuel cells can be used to generate simultaneously electric energy and useful industrial products. The present project examines the synthesis of hydrogen cyanide in zirconia cells with appropriate electrodes. A platinum electrode deposited on the outside wall of an yttria stabilized zirconia solid electrolyte is exposed to the ambient air. A platinum-rhodium electrode deposited on the inside wall is exposed to a CH_4-NH_3 mixture and serves as a catalyst as well. At 1 atm total pressure and temperatures about 1000°C oxygen passing through the O^{--} conducting solid electrolyte will oxidize the CH_4-NH_3 mixture to produce HCN and H_2O. In the same time the current produced will convert into electric power part of the free energy of the reaction. The primary goal is to establish optimal operating conditions for maximum HCN yield.

48. MULTIFUNCTION WALL SYSTEM FOR
APPLICATION WITH SOLAR HEATING
AND GROUND COOLING

VIRGINIA POLYTECHNIC INSTITUTE
AND STATE UNIVERSITY
Blacksburg, Virginia 24061

James F. Riley
College of Architecture & Urban Studies

Date Started: September 1, 1981

Funding: FY '84 $48,000 for 12 months

Anticipated Duration: 4 1/4 years

The purpose of this project is to conduct a program of research on an alternative energy building system concept which utilizes a multifunction wall system with solar heating and ground cooling. The concept of the building system is to expand the use of structure and enclosure elements of a building to function additionally as: the ductwork for the solar heated or earth cooled air, the heat transfer membrane between the heated or cooled air and the living environment of the building, the heat storage medium (in winter), and the temperature leveling and control medium. Activity in FY '84 will include the development of pilot building designs, testing of the existing experimental building with different floor massing, and testing of the durability of glass reinforced cement coatings as utilized in surface bonding cements and exterior insulation systems (critical components of the building system).

49.*A METHOD OF ACHIEVING SUPER-PRESSURES
BY ADVANCED GASDYNAMIC TECHNIQUES

UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

A. Hertzberg, A.P. Bruckner and Y.K. Rao
Aerospace and Energetics Research Program

Date Started: September 27, 1982

Funding: FY '83 $131,000 for 12 months

Anticipated Duration: 1 1/2 years

After a careful review of the theoretical analysis of the concept suggested in our original proposal, it was mutually agreed upon by the contract monitor and the principal investigator that the superpressure approach originally suggested and studied during the 1982-1983 contract period, did not offer sufficient advantages to warrant continuation. Therefore, the remaining funds in the project were re-directed towards alternate concepts which had emerged in preliminary form during the final phases of previous effort. The investigations resulted in the development of a novel approach whereby relatively large masses (several kg) could be accelerated using chemical energy to velocities in the 25 km/sec range. The availability of a technique which can accelerate large masses into this velocity range naturally suggested additional linear velocity multiplication to ultra velocities (100 km/sec range) and hence, formed the core of our remaining study effort. While the proposed new approach is not without problems, the potential efficiency and the ability to use chemical energy in a convenient form led to a series of theoretical studies which suggested that a thorough experimental exploration was warranted. In addition, due to the wide range of potential applications of this technique, this project has now been selected by the Air Force and DARPA for additional funding to carry out exploratory experimental studies. The investigators hope that this new approach will provide a way of accelerating masses of 10 g or more to ultrahigh velocities.

*Project completed

50.*ANALYSIS OF IMPACT FUSION TARGET DYNAMICS

UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

F.L. Ribe
Aerospace and Energetics Research Program

Date Started: April 15, 1983

Funding: FY '84 $111,000 for 12 months

Anticipated Duration: 3 years

In conjunction with rail-gun experiments on macroparticle acceleration we study the conversion of rectilinear projectile motion to a spherical or quasi-spherical implosion. Initial work involves one-dimensional numerical solutions of the hydrodynamic and transport equations, matched at the interface of a compressible metallic shell and an internal fusile gas for planar and spherical geometry. Present work also involves the two-dimensional problem of converting rectilinear to quasi-spherical particle and gas motion. In both cases, numerical hydrodynamic codes with particle and radiation transport have been written and applied to this problem. Analytical scaling estimates are compared with the numerical results.

*Projects 50 and 51 are cooperative interlaboratory projects.

51.*INVESTIGATION OF HIGH-VELOCITY ELECTROMAGNETIC LAUNCHER BEHAVIOR FOR USE IN IMPACT FUSION

WESTINGHOUSE R & D CENTER
1310 Beulah Road
Pittsburgh, Pennsylvania 15235

Y. Chia Thio
Electrotechnology Department

Date Started: July 18, 1983

Funding: FY '84 $386,000 for 12 months

Anticipated Duration: 4 years

In conjunction with impact fusion modeling study conducted at the University of Washington, Seattle, the present program is directed towards investigation of the scientific and technological problems associated with the electromagnetic acceleration of gram-size projectiles to ultrahigh velocity using a multi-stage distributed energy injection railgun. The major program milestones accomplished to date include the detailed design of the entire 84 ft multi-stage launcher, detailed design of the 24 MJ distributed energy capacitive pulsed power supply, development of an advanced simulation code for multistage launcher, the fabrication, assembly and testing of the launcher first stage (8 ft). Using only half the energy available for the first stage 1.2-g projectile was successfully accelerated to 5.1 km/s. In the second year of the program, extension of the launcher to 36 ft is planned. This will provide the opportunity to conduct launcher experiments upto approximately 20 km/s and associated high-pressure and high-velocity plasma studies.

*Projects 50 and 51 are cooperative interlaboratory projects.

SAMPLE

Statement of Work

1) Project Objective

The contractor shall investigate the electrocatalytic oxidative dehydrogenation of ethylbenzene and butane in solid electrolyte fuel cells. The effort is directed toward defining optimal operating conditions for achieving high yields of styrene and butadiene with simultaneous electric energy generation.

2) Scope of Work

The work to be performed consists of the following tasks:

2.1. Construction of tubular stabilized zirconia fuel cells with a platinum cathode and an iron oxide or platinum anode. Both anode materials are quite promising and a decision between the two will be made after preliminary runs.

2.2. Measurement of the styrene cell activity and yield as a function of temperature, inlet ethylbenzene concentration and external resistive load.

2.3. Measurement of the cell electric power output and overpotential as a function of the operating parameters described in 2.2.

2.4. Determination of the nature of the overpotential according to the results of 2.3. If ohmic overpotential dominates, a small well mixed cell with thin (150 microns) electrolyte discs will be constructed to increase power density.

2.5. Development of correlation for styrene yield and electrical power output in terms of operating and design parameters for use in future scale up.

2.6. Repeat tasks 2.2. through 2.5. using butane and/or butene as the fuel.

2.7. Preliminary engineering and economic analysis according to the results of 2.2. through 2.6.

3) Deliverables

The contractor shall provide the data of experiments performed according to paragraphs 2.2., 2.3., 2.4., 2.5. and 2.6 along with analyses and conclusions based on this data.

4) Performance Schedule

4.1. Complete construction of cells three months after start of work.

4.2. Complete ethylbenzene experiments within twelve months after start of work.

4.3. Complete butane and butene experiments and data analysis twenty months after start of work.

4.4. Complete data correlation, economic analysis and final report 24 months after start of work.

OFFICE OF BASIC ENERGY SCIENCES
DIVISION OF ADVANCED ENERGY PROJECTS

Fiscal Year 1984 Program Data

FY '84 Budget

Operating Funds............	$9,298,000
Capital Equipment Funds.....	$ 310,000

Distribution of Projects by Institutional Sector

Universities	40%
Small Business	27%
Other Industry	8%
DOE Laboratories	25%
	100%

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DOE/ER-0147/2

Annual Report and Summaries of FY 1984 Activities Supported by the Division of Biological Energy Research

October 1984

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Biological Energy Research
Washington, D.C. 20545

INTRODUCTION

Fiscal Year 1984 marked the fifth anniversary of the Division of Biological Energy Research (BER). The Division's program fulfills the need in the Department of Energy for a fundamental biological research activity designed to generate the information essential to development of biosystems related to energy matters. The research areas that the BER program supports are primarily in the bioconversion realm with primary emphasis on basic mechanistic studies.

In the five years of its existence, the BER program has been instrumental in enhancing the research activities in a number of specific areas of importance to the program. Most notable of these are: i) basic studies on methanogenesis, including the physiology, genetics and biochemistry of methanogens and of organisms that tie into the anaerobic digestion processes; ii) mechanisms of microbial breakdown of cellulose and other members of the lignocellulosic complex; iii) the plant cell wall, its structure and function; and iv) the biochemical changes associated with the responses of plants and microorganisms to physical stresses, temperature, moisture, pH and salinity.

Other major areas of emphasis in the botanical and microbiological areas, as will be noted on reading this report, include:

1) photosynthesis, the primary conversion of solar to chemical energy as carried on by green plants and bacteria.

2) the regulatory processes in growth and development of plants that determine ultimate productivity.

3) the metabolic regulatory mechanisms in plants that determine how the photosynthetic assimilated resources are utilized.

4) bioconversions by microorganisms involving fermentation mechanisms.

5) anaerobic and/or thermophilic microbial conversion mechanisms leading to materials useful as fuels or industrial chemicals.

6) the genetic and cellular processes that will serve as the foundation for genetic manipulation of plants and microorganisms in the future.

7) the basis of organismal interactions in symbiosis, host-pathogen and other interrelations with emphasis on recognition as well as information and metabolic transfer mechanisms.

The BER program is constantly evolving as the status of research problems changes, as new techniques and approaches to problems are developed, and in response to the changing perceptions of national research needs and opportunities.

Among the facets of the BER program that are considered of significance are the various efforts to improve or modify research techniques and tools for research in the plant and microbial sciences. This includes, where possible and appropriate, the employment of relatively sophisticated instrumentation to attack problems. In areas where the pool of available researchers is small, opportunities are provided for training. For example, BER has been providing support for introducing both undergraduate and graduate students to the intriguing world of the microbiology of non-medical anaerobic organisms, including microbial ecology, through the partial support of a summer research and training program at the Marine Biological Laboratory at Woods Hole, Massachusetts.

As has been the case since the beginning of the BER program, there has been an effort made to support, wholly or partially, workshops, symposia, and conferences on topics that are appropriate to the program. It is felt that such scientific meetings are critical for exchange of results and ideas, but, in addition, to provide forums to pursue topics in depth and to stimulate research and sometimes provide the setting for the generation of new approaches as well as for encouraging collaborations. The activities supported in FY 1984 included:

A) American Society for Microbiology - partial funding for a conference on "Genetics and Molecular Biology of Industrial Microorganisms" September 30-October 3, 1984, at Indiana University, Bloomington, Indiana.

B) University of California, Davis - partial funding of conference on "Molecular Basis of Plant Disease" August 19-23, 1984, at the University of California, Davis.

C) University of California, Davis - partial funding of conference on "Bicarbonate Utilization by Photosynthetic Organisms" August 18-22, 1984, at Asilomar Conference Center, Pacific Grove, California.

D) University of California, Riverside - partial funding for 7th Annual Symposium in Plant Physiology entitled "Structure, Function and Biosynthesis of Plant Cell Walls", January 12-14, 1984, University of California, Riverside.

E) University of Illinois, Urbana - partial funding of conference "Plasmids in Bacteria", May 14-18, 1984, University of Illinois, Urbana.

F) University of Minnesota - partial funding for "Implications of Molecular Genetics in Plant Breeding Symposium", June 4-6, 1984, University of Minnesota, St. Paul.

G) University of Tennessee - partial funding of "Plant Tissue Culture Symposium", September 9-13, 1984, University of Tennessee, Knoxville.

H) Cold Spring Harbor Laboratory - partial funding of a meeting on "Molecular Biology of the Photosynthetic Apparatus", May 9-13, 1984, Cold Spring Harbor, New York.

One particularly interesting and exciting workshop convened by BER was held 20-21 May 1984 to discuss the importance of complex carbohydrates in biological research and industrial processes. The principal focus was on analytical techniques for determining sequence and conformation of complex carbohydrates which are tremendously more difficult than analyses of either proteins or nucleic acids. The participants expressed the view that complex carbohydrates are being appreciated to have many more significant roles in biological function and in industry, (this recognition is expected to grow), and that structural information is now achievable with some very powerful and sophisticated, but expensive, techniques. The conclusion was that within the next few years, a small network of regional research and service centers for performing these analyses should be established. Such structural information should impinge on an extraordinarily broad array of disciplines and accordingly should stimulate the interest of many investigators in the scientific community.

Some representative contributions from investigators supported by BER funding may be highlighted:

a) Significant new insights about how gas exchange occurs in plants adapted to flooded conditions have been attained using deep water rice as a model. Leaf surface contours were shown to be critical for the diffusive transport of oxygen to roots while other reactions involving ethylene stimulated growth were demonstrated to be integrated into an adaptive pattern for adjusting to flooding stress.

b) The role of phosphorylated proteins in photosynthesis regulation is now much more evident as a result of some investigations on the control of the activity balance of the two photosystems in photosynthesis. The light harvesting chlorophyll a/b-protein complex appears to be phosphorylated by a kinase that is activated and deactivated depending on the oxidation-reduction state of the plastoquinone pool. This mechanism thus affords a more balanced distribution of excitation energy between Photosystems I and II.

c) During the course of the development of the microbial activity within an anaerobic digestor where methane gas is produced, it has been observed that the microbial populations change appreciably before stabilization is achieved. These dynamics have now been documented. The development of highly specific immunologic agents produced against various species of methanogenic bacteria has made identifications easier, faster and more reliable.

d) Working collaboratively with investigators in Belgium, one BER investigator has succeeded in the transfer of DNA coding for the synthesis of one of the major photosynthetic proteins (small subunit of ribulose 1,5 bisphosphate carboxylase) from one plant to another species of plant and having the message expressed. What is intriguing is that the DNA message transferred also contains coding for a light receptor that governs the development of chloroplast proteins. This finding affords new opportunities for studying developmental reactions that are controlled by light.

During FY 1984 the funds available to the BER program were distributed as follows:

	# of Projects	FY 84 Funding (in thousands of $)	% of Total Funds
University Contracts & Grants	83	5924	56
Michigan State University Plant Research Laboratory	11	1750	17
National Laboratories Brookhaven National Lab Lawrence Berkeley Lab Oak Ridge National Lab	12	2191	21
Solar Energy Research Institute	1	105	1
Other Research Institutions (federal, state, industrial, non-profit)	8	454	4
Conferences and miscellaneous	10	96	1
TOTAL	125	10520	

In FY 1984, a total of 86 new research proposals were received. Of these proposals, 15 were funded over and above the on-going projects. It must be pointed out that numerous fine proposals, judged to be worthy of funding in the review process, could not be accommodated into the program because of lack of funds. On-going projects are peer reviewed, usually on a three-year rotation and in competition with new proposals.

The proposal review process, site visit reviews, and other review activities in FY 1984 for the BER program involved over 550 scientists in this country and abroad. These individuals represented a broad cross section of disciplines as well as institutions. Without these many contributions by the research community, the BER program could not achieve and maintain the quality program that exists. For the many, many hours of effort that went into these reviews, we thank those involved most sincerely.

Any questions pertaining to the technical aspects of any research project should be addressed to the principal investigator.

Questions about the overall Biological Energy Research program should be directed to:

Dr. Robert Rabson
Division of Biological Energy Research
Office of Basic Energy Sciences, ER-17, GTN
U. S. Department of Energy
Washington, D. C. 20545
Phone: (301)353-2873

1. U.S. DEPARTMENT OF AGRICULTURE
Ithaca, New York 14853

REGULATION OF EXPRESSION OF A SOYBEAN STORAGE PROTEIN SUBUNIT GENE

$43,000

John F. Thompson and James T. Madison
Plant, Soil and Nutrition Laboratory

The goal of this research is to learn the mechanism by which added methionine turns off the expression of one soybean storage protein subunit gene. When immature soybean cotyledons are grown in organ culture, the addition of methionine to the culture medium prevents the appearance of the β subunit of the 7S storage protein. Cotyledon culture experiments have led to the following conclusions. First, the effect of methionine persists for at least three weeks. Second, the methionine effect is reversible since the β-subunit increased normally after removal of methionine. Third, methionine does not promote the degradation of the β-subunit. When methionine is present in the cotyledon culture medium, no translatable β-subunit mRNA is detected [Creason, Holowach, Thompson and Madison, Biochem. Biophys. Res. Commun. 117, 658-662 (1983)] indicating that methionine inhibits transcription or the processing of the initial transcript. Effects of methionine on translation or on the turnover of β-subunit mRNA appear to be minor. Hence the next step is to learn whether methionine inhibits transcription or a post-transcriptional modification of the initial transcript.

2. BATTELLE-C.F. KETTERING RESEARCH LABORATORY
Yellow Springs, Ohio 45387

THE BASIS FOR THE COMPETITIVENESS OF *RHIZOBIUM JAPONICUM* IN THE NODULATION OF SOYBEAN

$78,000

Wolfgang D. Bauer and William R. Evans

The objective of this research is to identify characteristics of the nitrogen-fixing bacterial symbiont, *Rhizobium japonicum*, which are crucial to its ability to compete effectively as a seed inoculant against indigenous rhizobia in nodulating the host plant, soybean. The ability of the bacterium to attach to the host root is likely to be an important characteristic with regard to both colonization of the root surface and the initiation of infections. The variables affecting root attachment capabilities are being determined. Attachment appears to be primarily mediated by bacterial pili (fimbriae) rather than binding of host root lectin. Antibodies against purified pili have been obtained and are being used to screen for mutants with altered attachment capabilities. Such mutants will be used to rigorously test the role of pili and attachment in competition. Quantitative nodulation assays have revealed that various strains of *R. japonicum* have markedly different efficiencies of nodulation, and that such efficiency depends on culture age. Various results indicate that nodulation efficiency, i.e. the number of bacteria required to generate a given number of nodules, may be related to synthesis of exopolysaccharide capable of binding soybean lectin. Transposon induced mutants of the bacteria are being screened for isolates incapable of synthesizing such polysaccharide in order to test this notion and its relevance to competition between strains. All *Bradyrhizobium* isolates tested thus far are able to remain viable and infective upon prolonged storage in "pure" water. We are seeking to identify the nutrients that support such viability to assess their use in inoculum preparation.

3. BOYCE THOMPSON INSTITUTE
Cornell University, Ithaca, New York 14853

CARBON METABOLISM IN LEGUME NODULES $42,000
Thomas A. LaRue

Symbiotic nitrogen fixation in legume nodules consumes more photosynthate than can be accounted for by the known energy requirements for nitrogenase. The object of our research is to determine how the legume nodule metabolizes carbohydrate to provide energy and reductant for nitrogen fixation. Because the plant cells within a nodule contain very little free oxygen, we are investigating the possible role of anaerobic pathways of carbohydrate metabolism.

We have established that plant enzymes characteristic of anaerobic metabolism do occur in nodules, and that the nodule contains low concentrations of alcohol and acetaldehyde. Both these carbon compounds can be used by the bacteroid to provide energy and reductant for nitrogen fixation.

Succinic acid is a major constituent of nodules, and is a substrate for the bacteroids. We are now determining if it synthesized by an aerobic or anaerobic pathway. We are studying the mitochondria isolated from nodules to learn how they function at the low concentration of oxygen. The oxidation and reduction of flavoproteins and pyridine nucleotides in intact mitochondria and bacteroids is monitored in situ by changes in their fluorescence.

4. BRANDEIS UNIVERSITY
Waltham, Massachusetts 02254

EFFECT OF LIGHT ON RESPIRATION AND DEVELOPMENT OF PHOTOSYNTHETIC CELLS $55,215
Martin Gibbs
Institute of Photobiology

One goal of this project is to determine the pathways of fermentation in algae with emphasis on organisms adapted to a hydrogen metabolism. The pattern of starch fermentation (mole product per mole glucose in starch consumed) in light vs dark is: ethanol 0.1, 0.9; acetate 0.0, 1.; formate 0.9, 2.1; CO_2 2.5,0; and H_2 6.9, 0.4. In light, DCMU decreases CO_2 and H_2, increases formate while having little effect on the other products or the rate of starch breakdown. Both the uncoupler, FCCP and DBMIB, an inhibitor of plastoquinone, doubles the rate of starch breakdown. The former increases acetate and H_2 photoevolution but not ethanol production while DBMIB increases ethanol production to 1.2 and reduces H_2 photoevolution. Alcohol and CoA dependent acetaldehyde dehydrogenases are found in cellular extracts. Light redirects C and H flow at the level of two carbon metabolism. In light, acetyl CoA is used anaerobically in biosynthesis: glycolytic NADH, the result of triose-P oxidation is channeled to plastoquinone and H_2 at the expense of ethanol and this route of chloroplast respiration is reversed by DBMIB removing the rate limiting step of pyridine nucleotide turnover. Isolated chloroplasts couple H_2 uptake to CO_2 assimilation (photoreduction) in the presence of DCMU at rates one-third of the parent cell. Photoreduction in contrast to photosynthesis is inhibited by rotenone suggesting that electrons from H_2, donated at the level of plastoquinone are required for photoreduction to occur. Current studies include enzyme profiles in order to determine if the fermentation sequence is chloroplast-localized and the pathways of H_2 in photoreduction and the oxyhydrogen reaction are also chloroplastically localized.

5. UNIVERSITY OF CALIFORNIA
Riverside, California 92521

CATALYTIC MECHANISM OF HYDROGENASE FROM AEROBIC N_2-FIXING MICROORGANISMS $45,000
Daniel J. Arp
Department of Biochemistry

This project deals with elucidation of the catalytic mechanism of hydrogenase from aerobic N_2-fixing organisms. Several properties of these hydrogenases make them ideal to function in an environment in which all of the available substrate is generated *in situ*, e.g., a very low rate of the back reaction, hydrogen evolution, and a low K_m for H_2. We are particularly interested in the enzyme from *Rhizobium*-induced root nodules because of the potential for increased legume productivity in symbioses expressing this enzyme. The specific goals of the proposed research are fourfold: to 1. determine the mechanism of the isotope exchange reaction of Rhizobial hydrogenase; 2. investigate Rhizobial hydrogenase catalyzed para-H_2 to ortho-H_2 conversion; 3. purify and characterize component 559-H_2 from soybean bacteroids and investigate its ability to couple to and form a complex with Rhizobial hydrogenase; and 4. purify and characterize the hydrogenase of *Azotobacter vinelandii*. The proposed research will provide insight into the mechanism of hydrogen uptake by Rhizobial and *Azotobacter* hydrogenase which, in turn, will lead to a better understanding of H_2 cycling in these organisms. This information is important to genetic engineering of new strains and may lead to improved techniques for selecting the best strains of *Rhizobium* for inoculation. The results may lead to new assays for hydrogenase activity and may provide new information about the structural organization of the bacteroid membrane. Our knowledge and understanding of hydrogenases in particular, and electron transferring proteins in general, should be significantly enhanced by these studies.

6. UNIVERSITY OF CALIFORNIA
Los Angeles, California 90024

ENERGY CAPTURE AND USE IN PLANTS AND BACTERIA $87,000
Paul D. Boyer
Department of Chemistry and Biochemistry and
Molecular Biology Institute

This study focuses on what is probably, quantitatively, the most important biological energy transduction in nature, namely the formation of adenosine triphosphate (ATP) by plants and bacteria. The formation of ATP by the membrane-bound ATP synthase complex is coupled to energy provided by light or by oxidation of metabolites. Our laboratory has had a leading role in developing an energy-linked binding change mechanism that appears to offer the best present model for how the ATP synthase functions.

Current hypotheses that are being explored are: 1) that energy serves to promote binding of ADP and P_i and release of ATP by the synthase, 2) that multiple catalytic subunits on the enyzyme participate in cooperative alternation, and 3) that during catalysis there is a rotational change in position of the catalytic subunits in relation to the noncatalytic core. In addition, we have proposed a new hypothesis for how energy transmission from electron-transport enzymes to the ATP synthase might occur.

We are undertaking studies with the chloroplast system on: The heterogeneity of conformation of the catalytic subunits; the nature of the Ca^{2+} as contrasted to Mg^{2+} activation; the spatial locations and reactivity of subunits during catalysis; which subunits are derivatized by inhibitors and substrate analogs; whether two or three catalytic sites operate in alternation; and finally, subunit positional interchanges by assessment of derivatization with fluorescent and related probes. With the *E. coli* ATP synthase we are studying the catalytic properties of mutant forms of the enzyme, to ascertain the function of various subunits by dissociation and reconstitution, and to develop methods for specific cross-links between subunits as tests for possible subunit spatial relationships during catalysis.

7. UNIVERSITY OF CALIFORNIA
Davis, California 95616

FLUORESCENCE PHOTOBLEACHING MEASUREMENTS OF PLANT MEMBRANE VISCOSITY: MECHANISMS OF RESISTANCE TO ENVIRONMENTAL STRESS

$60,000

R. W. Breidenbach, D. W. Rains, and M. J. Saxton
Plant Growth Lab/Agronomy and Range Science

The purpose of this project is to examine the role of the plasma membrane and tonoplast in determining the responses of different crop species to temperature and salinity: two factors strongly limiting plant productivity. The experiments use fluorescence photobleaching recovery to compare the lateral diffusion rates of proteins and lipids in the membranes of plants differing in their sensitivity to chilling temperatures or high concentrations of salts. Membrane viscosities of sensitive and resistant plants are being compared at various temperatures and salt concentrations. Since many important cellular processes may depend directly upon lateral motion of membrane proteins, this approach provides a direct measure of the relation between the physical properties of the membrane and plant responses to environmental stresses. Understanding of this relationship will provide useful strategies for developing tolerant new plant varieties for production of food, fuel and chemicals.

The techniques we will use will also enable us to examine two other problems in plant biophysics:

1) The effect of the cell wall on lateral diffusion rates
2) The mechanisms by which certain polysaccharide fragments trigger the synthesis by the plant of defensive compounds against fungal attack.

8. UNIVERSITY OF CALIFORNIA
Berkeley, CA 94720

THE REGULATION OF ENZYME SECRETION IN PLANT CELLS

$85,000

Russell L. Jones
Department of Botany

The aim of this project is to achieve an understanding of the events in cereal aleurone which are controlled by Ca^{2+} and to determine how this ion is metabolized. Our investigation of the control of hydrolytic enzyme synthesis and secretion focuses on α-amylase. α-Amylase is present in barley as four distinct isoenzymes, and we have shown that the *de novo* synthesis of two of these isoenzymes is controlled in part by Ca^{2+} and the plant hormone gibberellic acid (CA). We have prepared a cDNA clone from poly(A^{+})RNA isolated from aleurone layers treated with GA plus Ca^{2+} for 12h. We have characterized this clone and shown that it is complementary to RNA which codes for one of the α-amylase polypeptides whose synthesis is controlled by GA plus Ca^{2+}. We will use this cDNA clone to investigate the role of GA and Ca^{2+} in α-amylase gene expression. A project is also underway to prepare monoclonal antibodies to all four α-amylase isoenzymes. Although polyclonal antibodies have been raised to α-amylase, they cannot distinguish between closely related isoenzymes. Monoclonal antibodies will also be used to study the synthesis of barley α-amylase. We will isolate mRNA from aleurone layers incubated in the presence or absence of GA or Ca^{2+} and translate these mRNAs in vitro. The translation products will be identified using monoclonal antibodies. These experiments should pinpoint the site(s) where GA and Ca^{2+} control the *de novo* synthesis of α-amylase. Experiments are also in progress to study the metabolism of Ca^{2+}. We have shown that aleurone layers contain appreciable levels of Ca^{2+}(0.08% of aleurone dry weight). Eighty percent of this Ca^{2+} is bound to Ca^{2+}-binding ligands, but 20% is readily exchangeable. We are studying the metabolism of this pool with emphasis on its intracellular localization. The control of the transport of Ca^{2+} into and out of this pool is also under study.

9. UNIVERSITY OF CALIFORNIA
Irvine, California 92717
Berkeley, California 94720

BIOENERGETICS OF SALT TOLERANCE $142,000
Janos K. Lanyi
Dept. of Physiology and Biophysics, UC Irvine
Lester Packer
Dept. of Physiology and Anatomy, UC Berkeley

We are investigating the bioenergetics of salt tolerance with respect to ion transport across membranes, redirection of metabolic pathways for increased synthesis of osmoregulatory compounds, replacement of some salt sensitive components with salt resistant ones, and the signals which turn these processes on and off during salt stress. We have developed and adapted methods to study these phenomena mainly in two systems, each suited to answer specific questions. In the membranes of *Halobacterium halobium* and the cyanobacterium, *Synechococcus* 6301, we are studying the active and passive transport of sodium, potassium and chloride ions, and the regulation of the transporters. Particular attention is paid to sodium transport via a sodium/proton antiporter in the cyanobacterium, as related to adaptation to growth at low and high salinities. In the *Synechococcus* we explore also the cytoplasmic events which occur during short-term adaptation to salt. In the thylakoids of this organism we are attempting to describe features of the photosynthetic apparatus which are changed by salt stress. Results with these two systems so far have yielded interesting and promising results. Using this multi-organism approach, we intend to develop the conceptual basis for a refined description of the physiology of cellular and membrane adaptation to salt.

10. UNIVERSITY OF CALIFORNIA
Berkeley, CA 94720

THE RELATION OF ALLOZYME HETEROZYGOSITY TO GROWTH UNDER INBREEDING AND OUTCROSSING IN *PINUS ATTENUATA* $56,170
William J. Libby
Department of Forestry & Resource Management

The proposed study will investigate the significance of heterozygosity to components of fitness. It will study the relation of heterozygosity to growth in 10-year-old trees growing in plantations. Allozyme heterozygosity of selfed, outbred, and naturally pollinated trees will be related to their vegetative and reproductive rate of development. About 800 trees will be studied; their genotypes will be characterized for about 25 polymorphic enzyme loci. The project will test the hypothesis that heterozygosity promotes growth, fecundity, and developmental stability.

11. UNIVERSITY OF CALIFORNIA, LOS ANGELES
Los Angeles, California 90024

METHANOGENESIS FROM ACETATE, A KEY INTERMEDIATE IN NATURE

\$74,000

Robert A. Mah
Division of Environmental & Occupational Health Sciences
School of Public Health

The objective of this project is to study the H_2-oxidizing and methylotrophic methane-producing bacteria, especially aceticlastic methanogens from various naturally occurring anaerobic habitats. Enrichments for both H_2-oxidizing and methylotrophic methanogens were initiated by inoculating samples from widely varying environmental conditions such as sediments from the sulfuretums at Wadi el Natrun, Egypt and a solar saltern in Chula Vista, Ca. Substrates used in these enrichments included H_2/CO_2, methanol, acetate, and trimethylamine. The pH of the media corresponded to that of the inocula. For the Wadi el Natrun samples, the pH ranged from 7.3 to 9.5 and the salt concentration from < 1.0 to > 27%. The pH of samples from the saltern was ca. 7.3, and the salinity was near saturation. Vessels containing H_2/CO_2 as substrate produced methane more readily and more often than those with methylotrophic substrates. Methanogenic cocci, rods, and filamentous cells were presumptively identified by fluorescence at ca. 340 nm in both H_2/CO_2 and methylotrophic media. Isolation of these methanogens is now underway, and at least one of the Egypt samples will yield an axenic culture soon. Another strain of halophilic methanogen from the solar saltern is currently in co-culture and will also be obtained in axenic culture. Because of the unusual environmental conditions of the samples (pH, salinity), we expect to describe some new species of methenogens.

12. UNIVERSITY OF CALIFORNIA, SANTA CRUZ
Santa Cruz, California 95064

TONOPLAST TRANSPORT AND SALT-TOLERANCE IN PLANTS

\$60,000

Lincoln Taiz
Biology Department

Salinity (excess sodium chloride) is the most widespread limitation on crop productivity in the world today, yet many wild halophytic species, such as Salicornia and Distichlis, thrive under saline conditions. One of the distinguishing features of halophytes is their ability to take up sodium chloride into vacuoles, thus avoiding toxic effects on the cytoplasm. We are hypothesizing that the tonoplasts of halophytes may be specialized for transporting sodium, and that this property may reside in the tonoplast ATPase or in a specific membrane carrier protein. Our goal is to study the transport properties of purified isolated tonoplast vesicles from halophytic species, such as the grass, Distichlis, and to compare these properties with those of a nonhalophytic crop plant, Zea mays. Our studies indicate that the primary transport mechanism on the tonoplasts of corn is an electrogenic H^+-ATPase. Chloride ions are taken up by corn tonoplast vesicles in response to an inside-positive electrical potential generated by the proton pump. Detailed characterization of the transport properties of corn tonoplast vesicles will establish a basis from which comparisons with halophytes can be made. We are also purifying the H^+-ATPase for a detailed analysis of its structure and enzymatic properties. Preliminary results suggest that it is a multi-subunit enzyme having two major subunits with molecular weights of 70,000 and 60,000 daltons. Antibodies to these two subunits are being prepared, which will aid in the further purification of the enzyme. It is hoped that understanding the mechanism of ion transport across halophyte tonoplasts may one day allow salt tolerance to be introduced into crop plants by recombinant DNA techniques.

13. THE UNIVERSITY OF COLORADO
Boulder, Colorado 80309

STUDIES ON OLIGOSACCHARINS, CARBOHYDRATES POSSESSING BIOLOGICAL REGULATORY ACTIVITIES $116,690
Alan G. Darvill and Peter Albersheim
Department of Chemistry

This project entails identifying, isolating, and characterizing naturally occurring carbohydrates that possess biological regulatory activities. Such carbohydrates are called oligosaccharins. We observe that oligosaccharides, when released from the confines of the plant cell wall, regulate a variety of physiological functions in plants. More specifically, we are studying the purification and identification of (i) an oligosaccharin of plant cell wall origin that elicits phytoalexin (antibiotic) accumulation in plant tissues and that acts synergistically with a hepta-α-glucoside phytoalexin elicitor of fungal mycelial wall origin; (ii) an oligosaccharin, and enzymes involved in its metabolism, that inhibits 2,4-D-promoted growth in pea epicotyls and that may be involved in feedback control of auxin-stimulated plant growth; (iii) an oligosaccharin, hypothesized to be a trigger of the hypersensitive resistance response, that has been isolated from both monocot and dicot cell walls and that inhibits the incorporation of [^{14}C]leucine into proteins in both monocot and dicot cells; (iv) an oligosaccharin that inhibits flowering in duckweed (Lemna gibba G3) and tobacco cultures; (v) oligosaccharins that induce flowers, roots and vegetative bud primordia in isolated tobacco epidermal strips; and (vi) polysaccharides found in maple sap that indicate the presence of oligosaccharin-type molecules in the major conducting fluids of plants, molecules that, themselves, may have regulatory properties within plant tissues.

14. THE UNIVERSITY OF COLORADO
Boulder, Colorado 80309

STRUCTURAL STUDIES OF COMPLEX CARBOHYDRATES AND PLANT CELL WALLS $145,850
Michael McNeil, Alan G. Darvill and Peter Albersheim
Department of Chemistry

The cell wall is not only a determinant of structure and morphology of plants, but also a source of carbohydrates with biological regulatory functions and an important organelle in host-pathogen interactions. This grant funds our efforts to isolate and structurally characterize the complex carbohydrates that constitute about 90% of the walls of growing plant cells. Our research includes developing methods to purify and structurally characterize complex carbohydrates. Sources of the polysaccharides for this study include cell walls isolated from dicot, monocot and gymnosperm suspension-cultured cells and the extracellular polysaccharides secreted by these cells. The current foci of our research are a xyloglucan hemicellulose and two pectic polysaccharides: rhamnogalacturonans I and II. We have shown that these polysaccharides possess unexpectedly complex structures. RG-II, for example, contains at least 12 different glycosyl residues that include apiosyl, 2-O-methyl fucosyl, 2-O-methyl xylosyl, aceric acid (3-C-carboxy-5-deoxy-L-xylosyl) and KDO (2-keto-3-deoxy-manno-octonic acid). The structures of these polysaccharides are further complicated by the occurrence of O-acetyl esters on some of the glycosyl residues. We are developing methods to structurally characterize complex carbohydrates that include techniques to identify the exact locations of such O-acetyl and other base-labile substituents. We are also developing a procedure that employs lithium/ethylenediamine to degrade uronosyl residues in such a way that the neutral glycosyl residues of the polysaccharides remain intact. This method is particularly applicable to furthering the structural characterization RG-I and RG-II.

15. UNIVERSITY OF COLORADO
Boulder, CO 80309

THE GENETICS OF PATHOGENICITY OF THE *PYRICULARIA*

$87,570

Barbara Valent and Forrest G. Chumley
Department of Chemistry

The *Pyricularia* are important fungal pathogens of cultivated and wild grasses. Individual field isolates of *Pyricularia* infect one or a few different species of grasses. Rice-infecting isolatus exist as many races, defined by the variety of rice cultivars they can attack. A goal of this project is to conduct a genetic analysis of the differences in host specificity exhibited by various *Pyricularia* isolates. We have observed that field isolates of *Pyricularia* vary in fertility according to host range. Isolates pathogenic to goosegrass (*Eleusine indica*) have moderate fertility while those pathogenic to rice have very low fertility. We have increased the fertility of isolates that infect goosegrass by a systematic program of inbreeding and selection. These fertile laboratory strains are now being used in a program to develop fertile rice-infecting strains. Our program for improving fertility in *Pyricularia* field isolates has already led to the identification of *Pyricularia* genes that play a role in determining host specificity. For example, analysis of sexual crosses conducted between an isolate that infects goosegrass but not weeping lovegrass (*Eragrostis curvula*) and another isolate that infects weeping lovegrass but not goosegrass indicates that single gene differences control pathogenicity to each host species. In contrast, sexual crosses between rice-infecting strains and goosegrass-infecting strains reveal differences at several loci that determine the ability to infect rice. Among the rice-infecting progeny, we have detected a single gene that controls the ability to infect a rice cultivar that carries the resistance gene, Pi-ta. Molecular genetic analysis of these pathogen genes and others will lead us to an understanding of mechanisms determining host specificity of an important plant pathogen.

16. CORNELL UNIVERSITY
Ithaca, New York 14853

STUDIES OF PHOTOSYNTHETIC ENERGY CONVERSION

$35,927

Andre T. Jagendorf
Section of Plant Biology

Several species of unicellular marine diatoms are known to display considerable physiological plasticity with respect to their photosynthetic antenna size and composition in response to variations in growth irradiance. We propose to investigate the effects of ambient light intensity on the two major functions of antenna pigment-protein complexes: (1) efficient light harvesting and transfer of excitation energy to the photochemical reaction centers, and (2) control of the distribution of excitation energy between the two types of reaction centers. The light harvesting pigment-protein complexes of the diatoms *Phaeodactylum tricornutum* and *Skeletonema costatum* are being isolated by mild detergent treatment. The composition of these complexes is being analyzed with emphasis on the accessory pigments chlorophyll $\underline{c}_1$ and $\underline{c}_2$, and the carotenoids fucoxanthin, diadinoxanthin, and diatoxanthin. The relative antenna size of and efficiency of energy transfer to PSI and PSII are being estimated from the kinetics of P700 photobleaching and fluorescence induction, respectively. The kinetics of fluorescence induction and the reduction of the primary quinone acceptor of PSII (ΔA_{320}) are being measured simultaneously to assess the heterogeneity of PSII reaction centers. The control of excitation energy distribution between PSI and PSII is being investigated by observing slow changes in fluorescence yield and rate of oxygen evolution (State I - State II transitions) as a function of excitation wavelength. Through analysis of the effects of enhancement, the action spectra of PSI and PSII are being individually determined. In combination with measurements of pigment and reaction center concentrations, this allows the calculation of the number of each type of pigment molecule participating in PSI or PSII light harvesting. The influence of growth irradiance on chloroplast ultrastructure is also being investigated.

17. CORNELL UNIVERSITY
Ithaca, New York 14853

EFFECTS OF FREEZING AND COLD ACCLIMATION ON THE PLASMA MEMBRANE OF ISOLATED CEREAL PROTOPLASTS $63,100
Peter L. Steponkus
Department of Agronomy

The ultimate goal of this project is to develop a mechanistic understanding of cold acclimation and freezing injury to provide a basis for genetic engineering and traditional breeding studies for the improvement of plant cold hardiness and to provide for the formulation of effective protocol for the cryopreservation of plant germplasm. Cryomicroscopic observations reveal that destabilization of the plasma membrane can occur at various times during a freeze-thaw cycle and may be manifested as any one of several symptoms. In non-acclimated protoplasts, the predominant form of injury is expansion-induced lysis due to irreversible endocytotic vesiculation of the plasma membrane. Current studies of the mechanical properties and ultrastructural characteristics of the plasma membrane are directed to the formulation of a quantitative theory to explain membrane behavior during freeze-induced osmotic contraction/expansion and the influence of cold acclimation. A second form of injury is due to the loss of osmotic responsiveness following cooling and is associated with dehydration-induced lamellar to hexagonal$_{II}$ phase transitions in the plasma membrane. Current studies are directed to the influence of cold acclimation and carbohydrates on the incidence of these phase transitions. Both non-acclimated and acclimated protoplasts are subject to intracellular ice formation when cooled rapidly because mechanical failure of the plasma membrane results in seeding of the cytoplasm by extracellular ice. During rapid cooling, plasma membrane failure is associated with the generation of electrical fields during the freezing of the suspending medium. Current studies are directed to measurement of the spatial and temporal characteristics of the electrical field and the electrical properties of the plasma membrane. Isolation of purified plasma membrane vesicles has been completed. Compositional analyses are in progress.

18. CORNELL UNIVERSITY
Ithaca, New York 14853

THE IMPORTANCE OF PHYTOALEXIN TOLERANCE AND DETOXIFICATION FOR PATHOGENICITY. $59,297
Hans D. VanEtten and David E. Matthews
Department of Plant Pathology

The ability of plants to produce antimicrobial compounds (phytoalexins) in response to infection is believed to play an important role in preventing many microorganisms from causing disease. However, phytoalexin-producing plants are nonetheless susceptible to some diseases. Our research has demonstrated that one means by which successful pathogens overcome this potential resistance mechanism is by detoxifying their hosts' phytoalexins. The fungus *Nectria haematococca* can cause a root and stem rot of pea (*Pisum sativum*) even though the infected tissue accumulates high concentrations of the phytoalexin pisatin. Virulent isolates of this fungus detoxify pisatin by a demethylation reaction. In progeny of crosses between appropriate fungal isolates, pisatin demethylation segregates as an essential trait for virulence on this host. We have recently found that *N. haematococca* possesses at least 4 independently acting genes for pisatin demethylation. Two of these genes confer only low rates of demethylation, and do not enhance virulence toward pea. We are currently working to determine the relationship between these genes and the enzyme pisatin demethylase. The enzyme activity in one highly virulent, rapidly demethylating isolate of the fungus has been characterized as a substrate-inducible microsomal cytochrome P-450 monooxygenase. The two required components, NADPH-cytochrome c reductase and cytochrome P-450, have been solubilized and resolved chromatographically. Further purification is underway. Data on the substrate specificity and inhibitor sensitivity of this enzyme are also being collected. Comparison of the physical and catalytic properties of this enzyme with the properties of pisatin demethylase preparations from other isolates of known genotype will help test the hypothesis that *N. haematococca* possesses multiple structural genes for pisatin detoxifying enzymes.

19. CORNELL UNIVERSITY
Ithaca, New York 14853

STUDIES OF THE GENETIC REGULATION OF THE *THERMOMONOSPORA* CELLULASE COMPLEX

$60,277

David B. Wilson
Department of Biochemistry, Molecular and Cell Biology

The goal of this project is to construct recombinant organisms which overproduce the most active cellulases produced by the thermophilic bacterium, *Thermomonospora YX*. Enzymatic screening of *E. coli* cells transformed by two different *Thermomonospora* gene banks has identified two genes which produce proteins with CMCase activity. Neither of these genes codes for a major *Thermomonospora* cellulase. *E. coli* clone banks will be screened using an antiserum against *Thermomonospora* culture supernatant that reacts with the major cellulases. Any clones which are positive in this screening will be tested using the specific antisera prepared against each purified cellulase that has been made. If this method fails, then gram positive organisms will be used to construct a *Thermomonospora* gene bank, which will be screened for the ability to make cellulase and the ability to make proteins which react with the antibody. The originally isolated cellulase gene is also being subcloned to construct *E. coli* strains which overproduce this enyme. Once the best method for doing this is found, it will be used to construct strains which overproduce any major cellulase genes which are isolated. In addition to constructing strains which overproduce cellulases, attempts will be made to construct strains which can grow on cellulose. If these are constructed, they will be used to try to isolate mutant cellulases which are resistant to inhibition by cellobiose by direct selection of mutagenized cells on plates containing cellulose and cellobiose.

20. CORNELL UNIVERSITY
Ithaca, New York 14853

MICROBIAL ECOLOGY OF THERMOPHILIC ANAEROBIC DIGESTION

$68,083

Stephen H. Zinder-
Department of Microbiology

The objective of this project is to provide an integrated understanding of the ecology of the microbial populations in a thermophilic (58°C) laboratory-scale digestor being fed a lignocellulosic waste. Among the methods being used to study these organisms are: 1) viable counts and culture studies using habitat and niche simulating media; 2) direct microscopic observation of populations using phase-contrast, epifluorescence, and electron microscopy; and 3) ^{14}C-radiotracer methods to study carbon flow to methane and physiological ecology of the digestor populations. Results obtained thus far include: 1) the apparent displacement of *Methanosarcina* by a previously undescribed thermophilic *Methanothrix* as the dominant aceticlastic methanogen in the digestor. A culture of this *Methanothrix* is now isolated and is currently being characterized; 2) the co-isolation of a two-membered coculture which converts acetate to methane using interspecies hydrogen transfer; 3) the demonstration that the overall temperature responses of the digestor are greatly dependent on the temperature responses of the dominant aceticlastic methanogen; 4) the demonstration that when *Methanothrix* was numerous in the digestor that methanogenesis from acetate was the process most easily saturated; and 5) the development of a method to enumerate autofluorescent methanogens in the digestor sludge. Current research centers on studying carbon flow to methane using an HPLC system to fractionate ^{14}C-label, and studies on improving digestor startup by adding specific methanogenic cultures.

21. DESERT RESEARCH INSTITUTE, UNIVERSITY OF NEVADA
P.O. Box 60220, Reno, Nevada 89506

GAS EXCHANGE CHARACTERISTICS OF LEAVES AND THE BIOCHEMICAL REACTIONS LIMITING PHOTOSYNTHESIS — $42,100
Thomas D. Sharkey
Biological Sciences Center

The objective of this research is to characterize the outward manifestations of various limitations on the instantaneous rate of photosynthesis in intact leaves. A specially constructed high speed freeze clamp-gas exchange chamber will be used to take samples of leaves whose gas exchange characteristics have been determined. These experiments will test predictions made by recent models of photosynthesis and identify those areas where our understanding of photosynthesis is incomplete. Particular attention will be paid to the biochemical limitation that occurs in plants growing under optimal conditions. Current indications are that the capacity of plants for triose phosphate utilization (TPU) can impose a limit on the rate of photosynthesis. TPU limited leaves are being studied by gas exchange analysis (especially for oxygen sensitivity), by metabolite analysis of rapidly frozen leaves, and by room temperature steady state fluorescence. The pool size of orthophosphate (P_i) inside the chloroplast will be measured and the P_i metabolism modeled to see how the P_i level changes during the TPU limitation and whether modification of P_i metabolism would result in plants with a higher capacity for photosynthesis. These studies are intended to determine the importance of the TPU limitation to photosynthesis rates and explore the interface between photosynthesis in chloroplasts and the physiology of the rest of the plant.

22. FLORIDA STATE UNIVERSITY
Tallahassee, Florida 32306

GUARD CELL BIOCHEMISTRY — $85,000
William H. Outlaw Jr.
Department of Biological Science

Most H_2O and CO_2 exchange between a leaf and the atmosphere is controlled by stomatal aperture size. Thus, when the surrounding guard cell pair accumulates potassium salts, these cells become more turgid and the pore enlarges. The current aperture size is a compromise between the opposing priorities of preventing dessication and satisfying the demand for CO_2. Typically, many environmental factors are integrated to effect this compromise. The immediate goal of this project is to identify correlations between metabolic events in guard cells and environmental pertubations that affect gas exchange. Because guard cells are sprinkled about in the leaf epidermis, special techniques for their study are necessary. We take three approaches for obtaining pure samples of *Vicia faba* guard cells: (1) protoplast isolation, (2) dissection of guard cells from frozen-dried leaves and (3) dissection of live guard cells from epidermal peels. In brief, our current work is in the following areas: (1) quantitation of [ABA]* in guard cells and other leaf cells (in collaboration with J. Zeevaart) using physico-chemical analysis; our preliminary results indicate that stressed guard cells accumulate ABA; (2) quantitation of [ABA] in guard cells by ELISA. Unfortunately, our monoclonal lines against ABA-protein are not stable. Thus, we are immunizing rat and rabbit in an attempt to develop polyclonal antibodies; (3) development of techniques for *real-time*, *direct* assay of enzyme activity in single cells using *natural* substrates. This project is virtually completed and its potential impact in many areas of biological research is significant; (4) *in vivo*, quantitative assay of NR in guard cells. *In vivo* assay, though more difficult, is considered necessary because of the lability of extracted NR. Preliminary results with small tissue slices (~100 cells) indicates that necessary miniaturization is feasible.

*ABA - abscisic acid

23. UNIVERSITY OF FLORIDA
Gainesville, Florida 32610

INVESTIGATION OF THE TRANSPOSITION OF MITOCHONDRIAL DNA AND ITS RELATIONSHIP TO FERTILITY IN ZEA MAYS
Rusty J. Mans
Department of Biochemistry and Molecular Biology, J-245
JHMHC

$58,245
(FY 83)

We are looking for altered expression of mitochondrial genes that affect male fertility in maize. These genes are rearranged and their copy number altered upon the spontaneous reversion of an S-type cytoplasmically male sterile parental plant to fertility. Sterility in these lines is also suppressed or repressed by the dominant allele of a nuclear gene, i.e. restorer to fertility (Rf3). We have cloned segments of the transposable mitochondrial genes into pBR322 for use as templates in an in vitro transcription system. We have purified an alpha-amanitin sensitive RNA polymerase from maize seedlings that transcribes inserted maize mitochondrial DNA sequences more efficiently than those of the vehicle. We have prepared polyclonal antibody to the RNA polymerase preparation as a tool for recognizing and isolating a putative maize DNA recognition factor in the polymerase preparation. We are attempting to couple the catalytic activity of a pure maize poly A polymerase with that of maize RNA polymerase using the defined templates. We are characterizing the products that accumulate and that hybridize with the maize DNA inserts to ascertain the specific "start" and "stop" signals recognized by the maize polymerases. These results will facilitate the use of portions on the mitochondrial genome as putative vehicles for genetic engineering of this agronomically significant crop.

24. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

ROLE OF CA^{2+} AND CALMODULIN IN PHOSPHORYLATION OF PROTEINS IN PLANTS
Milton J. Cormier and Alice C. Harmon
Department of Biochemistry

$65,000

The long-range goal of this project is to understand the molecular basis by which plant cells respond to external stimuli such as light, temperature changes, growth regulators, etc. The evidence to date suggest that many regulatory processes in plant cells are mediated through stimuli-induced changes in the intracellular levels of free Ca^{2+}. One of the cellular targets for Ca^{2+} has been identified by us as the Ca^{2+}-binding protein, calmodulin. Furthermore, we have shown that the calmodulin-Ca^{2+} complex is required for the activation of plant NAD kinase which regulates the NADP/NAD ratio. We are currently focusing on regulatory processes which are mediated via Ca^{2+}-dependent protein phosphorylation. We have observed Ca^{2+}-dependent protein kinase activity in the supernatant and membrane fractions obtained from a soybean cell line grown in suspension culture. A number of endogenous protein substrates were phosphorylated in the presence of gamma labelled ^{32}P-ATP. Following SDS-PAGE of the precipitated proteins, autoradiograms of the stained gels revealed the presence of about 20 phosphorylated polypeptides of which about half were phosphorylated in a Ca^{2+}-dependent manner. The purification and characterization of these enzymes and some of their substrates are in progress and represent a first step in understanding the role of protein phosphorylation in plants.

25. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

BIOSYNTHESIS OF A MICROBIAL BIOSURFACTANT $83,790
W. R. Finnerty and Mary E. Singer
Department of Microbiology

The goals of this project are to determine the genetic and biosynthetic mechanism(s) of glycolipid synthesis by a gram-positive microorganism. This product is an extracellular biosurfactant effective in the reduction of viscosity of heavy crude oils and displacement of oil from inert matrices. We are isolating mutants defective in fatty acid degradation, alkane utilization and glycolipid biosynthesis to determine the genetic relationship between glycolipid synthesis and alkane oxidation. Growth of the organism on alkane represents an obligate prerequisite for the synthesis of biosurfactant. We have determined that arsenate-resistance is plasmid-encoded in this organism. This trait is being used to cure the organism of 55-, 14.5- and 11.5 Mdal plasmids and to determine the relationship of plasmid-localized genes to alkane oxidation. Several arsenate-sensitive, hexadecane-negative strains have been recovered following sodium dodedecyl sulfate curing procedures. Enzyme studies have demonstrated the presence of cell-localized esterase and lipase plus a cellular and extracellular acyl transferase. The relationship of these enzymes to glycolipid synthesis, modification or release to the growth medium is being investigated. Current results indicate an excess carbon/limiting nitrogen imbalance stimulates extracellular glycolipid synthesis with maximum extracellular glycolipid synthesis correlating to the stationary growth phase and an external nitrogen concentration of 4 mM. Current studies are directed to determining specific enzymes induced by growth on alkane and the precursor relationship between cellular glycolipid and extracellular glycolipid with respect to biosynthesis, modification and release from the cells.

26. UNIVERSITY OF GEORGIA
Tifton, Georgia 31793

DEVELOPMENT OF INNOVATIVE TECHNIQUES THAT MAY BE USED AS MODELS TO IMPROVE PLANT PERFORMANCE $36,000
Wayne W. Hanna and Glenn W. Burton
Department of Agronomy

The objectives of this project are to develop techniques for transferring genes from wild species to cultivated plant species, to demonstrate the wealth of germplasm in the secondary and tertiary gene pools that can be transferred to cultivated species and to develop an obligate apomictic pearl millet. Species within the genus *Pennisetum* are being used as test organisms. The approach utilizes plants of wild species with different genetic backgrounds and ploidy levels (chromosome numbers) crossed and back-crossed with different genotypes of pearl millet, *P. americanum*, with different ploidy levels to produce fertile interspecific hybrids and derivatives. This research has shown how valuable germplasm can be masked on certain genomes by other genomes and 'stored' in a perennial or vegetatively propagated wild species such as *Pennisetum purpureum*. We have been able to transfer this 'hidden' or 'stored' germplasm to cultivated pearl millet and are in the process of evaluating it. Partially fertile and apomictic BC$_1$ pearl millet x *P. squamulatum* hybrids have been produced showing the potential of transferring apomixis from the wild to cultivated species to fix hybrid vigor. Diverse cytoplasm from the wild species have been transferred to pearl millet and are in the initial stages of evaluation. The overall impact would be on increased, more efficient and more reliable production of food, fiber, and forage.

27. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

ENVIRONMENTAL STRESS MEDIATED CHANGES IN TRANSCRIPTIONAL AND TRANSLATIONAL REGULATION OF PROTEIN SYNTHESIS IN CROP PLANTS

$86,520

Joe L. Key
Department of Botany

When soybean seedlings are subjected to an immediate shift from 30° to 40° or to a gradual (e.g. 3° per hr) increase to 40° to 45° there is a dramatic and rapid shift in the pattern of protein synthesis. Most normal protein synthesis rapidly declines at a temperature of about 40° and a new set of proteins (hsps) is rapidly induced. The synthesis of hsps correlates with the rapid induction, detectable within 3 to 5 minutes, of hs-specific RNAs encoding a complex set of 30 to 40 polypeptides. These sequences subsequently accumulate to as many as 20,000 copies per cell. The system appears to be self-regulated since it "turns off" after 6 to 8 hr of continuous hs, indicated by the depletion of hs mRNAs, cessation of hsp synthesis, and the resumption of normal protein synthesis. This "turn off" occurs more slowly during prolonged high temperature treatment than when the seedlings are returned to 30° after a short, 2 to 4 hr hs at 40°.

One putative function of hs proteins is a role in the development of tolerance to high temperatures through a conditioning treatment at a lower, hsp inducing temperature. An initial hs treatment (e.g. 2 hr at 40° or 5 to 10 min at 45° followed by 2 hr at 30°) provides thermoprotection to a subsequent, otherwise lethal temperature (e.g. 2 hr at 45°). This short-term thermal adaptation correlates with the accumulation of hsps and their selective localization during hs. A wide range of plant species are known to synthesize a complex group of hsps. There is considerable variation in the electrophoretic pattern of the 15 to 27 kD hsps, while the high molecular weight hsps are highly conserved. Although many stress agents induce low levels of hs mRNAs based on Northern hybridization analyses using hs cDNA clones to probe poly(A)RNAs from tissues stressed by other agents, only arsenite treatment closely mimics hs, as evidenced by intense radiolabeling of hs proteins. Cadmium also induces a small subset of the hs proteins and hs mRNAs. The hs genes comprise several multigene families, probably with over-lap among these families, as analyzed by Southern hybridization, 2D gel analyses of hybrid-selected translation products, and DNA sequence analysis of cDNA and genomic clones.

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28. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

SOYBEAN RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL SUBUNIT GENE FAMILY: GENE STRUCTURE AND REGULATION OF GENE EXPRESSION

$73,000

Richard B. Meagher
Department of Genetics

The goal of this research has been to determine the mechanism of the regulation controlling the transcription of the nuclear-encoded ribulose bisphosphate carboxylase small-subunit (RuBPCss) gene family in soybean. Although the soybean gene family contains 8-12 members, we have focused our attention on two unlinked but closely related pairs of genes, SRS1 and SRS2. The steady state levels of poly A+ transcipts from both genes are very high in light-grown leaves and shoots and at least 50 to 100 fold lower in dark-grown leaves and shoots. We estimate that message levels may range from 0.2% in the dark to 2% of the poly A+ mRNA in the light. To determine the manner in which the mRNA levels were controlled, we assayed the transcription rates for these genes in isolated nuclei under a variety of light and dark conditions. In summary, these genes can show a slight (2-4 fold) transcriptional induction in as little as 30 minutes after dark-grown seedlings are exposed to light. Maximum transcriptional induction takes between 24 and 48 hours of light. In light pulse experiments, where plants are exposed to only short periods of light and then returned to the dark before assaying for transcriptional levels, 10 minutes of white light can lead to a 10 fold induction of transcription five hours later. If white light is followed by 10 minutes of far red light, little or no transcriptional induction is observed. These results confirm that phytochrome is involved in transcriptional control of these genes. We will continue to analyze the transcriptional regulation of the members of the small subunit gene family in soybeans. We have just begun to use these strong control signals to direct the transcription of foreign genes in plants.

29. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

THE MICROBIOLOGY AND PHYSIOLOGY OF ANAEROBIC FERMENTATIONS OF CELLULOSE $220,000
Harry D. Peck, Jr. and Lars G. Ljungdahl
Department of Biochemistry

Investigations into the biochemistry and physiology of the four major groups of microorganisms (primary, ancillary, secondary and methane bacteria) involved in the anaerobic conversion of cellulose to methane and carbon dioxide will be continued. Studies on the primary or cellolytic microorganisms will be focused on the isolation of new thermophilic strains from Iceland, interactions with ancillary bacteria which ferment cellobiose and xylose, growth and modification of fermentation patterns by inorganic pyrophosphate and purification of cellulase. The projected investigations of the ancillary bacteria will emphasize isolation of new strains and increasing ethanol production with T. ethanolicus. The latter research will involve genetic modifications, enzymological studies on the regulation of appropriate enzymes and a study of the effect of inorganic pyrophosphate on growth and fermentation patterns. The enzymology of acetate formation from carbon dioxide by acetogenic bacteria will be studied with initial emphasis on the metabolism of the one-carbon compounds. Further studies with these organisms will include bioenergetics, especially hydrogen metabolism and energy coupling by H_2 cycling, and the structure and function of electron transfer components. Research on secondary bacteria will emphasize the sulfate reducing bacteria from the aspects of H_2 cycling, specificities of electron transfer proteins and enzymes, the mechanism of bisulfite reductase and APS reductase and the enzymology and physiology of both H_2-utilizing and acetate utilizing methanogens will continue to be investigated. The studies with H_2-utilizing methanogens will stress hydrogenase and the effect of inorganic pyrophosphate on growth. The research on the acetate-utilizing methanogens will involve the bioenergetics of sulfite reduction and the mechanism of acetate formation induced by pyrophosphate.

30. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

PHYTOCHROME PROPERTIES AND FUNCTION IN PHOTOSYNTHETICALLY COMPETENT PLANTS $50,319
Lee H. Pratt
Department of Botany

Plants respond, via the chromoprotein phytochrome, to the wavelength distribution of incident radiant energy in ways that alter both photosynthetic productivity and the partitioning of photosynthetically fixed carbon within the plant. In part because of the low abundance of phytochrome in green plants, however, almost nothing is known about the molecule as it exists in them. As a first step towards understanding how phytochrome modulates primary plant productivity, therefore, the properties of this pigment as it exists in green, photosynthetically competent tissues is being investigated, with a focus on two plants of agronomic importance: oats (Avena sativa L.) and peas (Pisum sativum L.). Polyclonal and monoclonal antibodies to oat and pea phytochromes, both of which were purified from etiolated tissues, are being produced and used to quantitate, visualize, and characterize phytochrome from green plant tissues. While developing and using an enzyme-linked immunosorbent assay that is sensitive to picogram (subfemtomol) levels of phytochrome, it became evident that phytochrome from green plants is antigenically distinct from phytochrome isolated from etiolated, but otherwise identical, plants. This antigenically unique phytochrome is being characterized, not only to determine whether it might arise from some artifact, but also to learn how it differs from the pigment as isolated from etiolated tissue. To achieve these goals, all currently available monoclonal antibodies to phytochrome (about 40 at present) are being screened to determine which of them bind to phytochrome from green plants and to which part of the phytochrome molecule they bind. Monoclonal antibodies that are specific to epitopes on phytochrome from green plants will, if possible, be made in the near future to permit its selective immunopurification, immunoquantitation, and immunovisualization.

31. THE UNIVERSITY OF GEORGIA
Athens, Georgia 30602

NITROGEN CONTROL OF PHOTOSYNTHETIC PROTEIN SYNTHESIS — $65,000
Gregory W. Schmidt
Department of Botany

The detrimental effect of nitrogen deficiency on photosynthetic carbon metabolism is a major limitation to plant growth and productivity. Photorespiratory assimilation of oxygen by ribulose 1,5-bisphosphate carboxylase/oxygenase (RuBPCase) results in a severe loss of reduced carbon when ammonium is not readily available. Nitrogen also influences photosynthetic efficiency by affecting the levels of chloroplast proteins. Our research concerns the molecular basis of the nitrogen regulatory process in photosynthetic cells. As a model system, we employ the unicellular alga *Chlamydomonas reinhardtii* grown in a continuous culture system in which nitrogen provision is precisely controlled. This enables high resolution analyses of the status of the photosynthetic apparatus in nitrogen limited cells and the molecular consequences of nutrient repletion. The major proteins whose levels are regulated by nitrogen are RuBPCase and the apoproteins of thylakoid membrane light-harvesting complexes. Immunochemical analyses show these proteins are preferentially reduced when the cells are grown in nitrogen-limiting conditions. With antibodies against seven other proteins we have determined that nitrogen differentially regulates the accumulation of the alpha and beta subunits of the photosynthetic ATP synthetase, the apoproteins of Photosystem I and II reaction centers, a core protein of PS II, a protein of the water oxidation complex and plastocyanin. In vivo pulse-chase labeling studies establish the effects of nitrogen on the rates of synthesis and turnover of these and other cellular proteins. Assays of mRNA abundance have revealed that some nitrogen-regulated proteins are strongly regulated at a transcriptional level. Detailed studies are in progress to resolve the means by which nitrogen profoundly affects expression of both nuclear and chloroplast genes that encode some, but not all, photosynthetic proteins.

32. UNIVERSITY OF GEORGIA
Athens, Georgia 30602

THEORY ON EXTREME THERMOPHILIC ANAEROBES GROWING OVER TEMPERATURE SPANS OF 40°C OR MORE. — $40,000
Juergen K. W. Wiegel
Department of Microbiology

Bacteria that grow over 70°C are considered extreme thermophiles. Among these, there are species able to grow over an extended temperature span of 40°C or more. Examples for this group are the anaerobic eubacteria *Clostridium thermohydrosulfuricum*, *Thermoanaerobium brockii*, *Thermoanaerobacter ethanolicus*, the anaerobic archaebacterium *Methanobacterium thermoautotrophicum* as well as the aerobic *Bacillus stearothermophilus*. They all grow in the temperature range of approximately 35 to 78°C. For these species we have shown that they exhibit a biphasic dependence of the growth rate (or other growth parameters) and the growth temperature. The corresponding Arrhenius graph has a curve with an intermediary plateau, which, depending on the organism, can be very distinct or only minor. The plateau is found between 55 and 60°C. This biphasic growth response will be investigated on the enzyme (protein) level by examining the protein pattern of the organisms grown at various temperatures including T_{min}, T_{opt}, and T_{max}, below, at, and above the plateau. Initially we will use two dimensional gel electrophoresis (O'Farrell's gel) to obtain the differences in protein pattern related to growth temperatures. These experiments will be followed by temperature shifts with the employment of radioactive labeled amino acids. These studies will reveal whether a synthesis of new proteins occurs in bacteria when shifting the growth temperature from below to above that of the plateau. This is done to evaluate the forwarded hypothesis: that these organisms inherit, for some critical enzymes/proteins, two sets of proteins: one for the lower range of 35 to approximately 65°C and one for the upper temperature range from around 50 to 78°C.

33. GRAY FRESHWATER BIOLOGICAL INSTITUTE
Navarre, Minnesota 55392

PHYSIOLOGY AND GENETICS OF METHANOTROPHIC BACTERIA
R.S. Hanson
Gray Freshwater Biological Institute/University of Minnesota
$44,761

The objectives of this project are to develop techniques for genetic studies of the regulation one-carbon metabolism in bacteria that utilize one carbon compounds. Because these bacteria are resistant to many antibiotics used as markers on plasmids employed for genetic engineering of gram negative bacteria and are not transformed by these plasmid DNA's we have constructed new cloning vectors with the following properties. The vectors contain resistance markers for kanamycin and tetracycline and can be transferred between Pseudomonas aeruginosa, Escherichia coli and several methylotrophs by conjugation. The vectors contain a cos gene that permits recombinant (vector/DNA) molecules to be packaged into bacteriophage lambda. The bacteriophage, constructed in vitro, is used to transfer hybrid DNA into E. coli. Clones containing genes encoding seven enzymes for the catabolism of methanol assimilation of formaldehyde have been identified in clones by complementation of mutations in methylotrophs after mating with clones in the E. coli genomic library. These genes have been mapped on five different 50 kbp DNA fragments. The gene encoding the large molecular weight (60,000) subunit of methane monooxygenase from a type II methylotroph has also been cloned. The clones carrying this gene have been identified using antibodies prepared using the pure protein as an antigen. Current studies are directed at precisely mapping genes involved in C_1 metabolism and cloning the promoter for the gene encoding the methane monooxygenase. This protein represents about 20% of the total cellular protein and the gene appears to be present in a single copy in the cells. We have also isolated and completed a restriction map of a 125 kbp plasmid from a type II methylotroph. This plasmid is transferred by conjugation to Ps. aeruginosa and is capable of mobilizing chromosomal genes from Organism SB1.

34. HARVARD UNIVERSITY
Cambridge, Massachusetts 02138

UNRAVELING PHOTOSYSTEM II
Lawrence Bogorad
Department of Cellular and Developmental
Biology
$80,000

The prokayotic cyanobacteria and eukaryotic higher green plants carry out basically the same type of oxygen evolving photosynthesis. Since some species and strains of cyanobacteria can be transformed with foreign DNA, they are suitable organisms for molecular biological analyses of the photosynthetic apparatus. The current focus of this project is on using cloned characterized maize chloroplast genes for components of the photosynthetic apparatus to identify and isolate the comparable genes from banks of clones of DNA prepared from two species of cyanobacteria that can be transformed. The maize chloroplast genes we have tested hybridize to the cyanobacterial DNA and permit us to identify the corresponding cyanobacterial genes. These genes, in variously modified forms, are to be reintroduced into the cyanobacterium in order to identify particular photosynthetic functions with segments of the protein for which the gene codes.

35. HARVARD UNIVERSITY
Petersham, Massachusetts 01366

STRUCTURE AND FUNCTION OF FRANKIA VESICLES IN DINITROGEN FIXATION BY ACTINORHIZAL PLANTS — $72,852
John G. Torrey
Cabot Foundation, Harvard Forest

Frankia, a filamentous bacterium which induces N_2-fixing root nodules on the roots of a wide range of woody dicotyledonous plants, is the first known actinomycete which fixes dinitrogen when growing in free-living pure culture. The nitrogenase enzyme is induced in many strains of this organism by withholding fixed nitrogen compounds from its nutrient medium. Terminal swellings of the bacterial filaments develop rapidly and acetylene reduction activity (= nitrogenase) increases in proportion to the number of terminal vesicles formed. The induction of vesicles and establishment of acetylene reduction occurs under aerobic conditions and the evidence is accumulating which demonstrates the existence of a multilaminate vesicle envelope which serves as a physical barrier protecting the oxygen-labile nitrogenase from denaturation. Our studies are concerned with the physiology, biochemistry and structural development of the N_2-fixing apparatus in Frankia grown in vitro and in root nodules of host plants. Diverse strains of Frankia are under study isolated and cultured from different host plants. Two strains have been studied especially HFPArI3, an isolate from nodules of the red alder Alnus rubra and HFPCcI3 isolated from root nodules of the tropical tree Casuarina cunninghamiana. The goal is to understand the structure and function which leads to optimum effectiveness for dinitrogen fixation.

36. UNIVERSITY OF IDAHO
Moscow, Idaho 83843

GENETICS AND CHEMISTRY OF LIGNIN DEGRADATION BY STREPTOMYCES — $73,000
Don L. Crawford
Department of Bacteriology and Biochemistry

The objectives of this research are to chemically characterize the intermediates of lignin degradation by Streptomyces, and to develop genetic techniques for manipulating and characterizing the lignin-degrading enzyme systems of these microorganisms. We are isolating and quantifying important lignin degradation intermediates, particularly water soluble, modified lignin polymers produced by Streptomyces strains. We are also examining and comparing the chemistry of modified lignin polymers produced by different Streptomyces as they decompose lignins. Enhanced lignin degrading strains are being isolated using ultraviolet irradiation mutagenesis, and by gene amplification using the recombinant DNA technique protoplast fusion. Protoplast fusions include interspecies crosses between different ligninolytic Streptomyces and intraspecies self fusions between protoplasts from a single species. Stable strains which overproduce polymeric intermediates have now been obtained using both mutagenesis and fusion. The chemistry of the intermediates generated by mutants and recombinants is now being examined and compared with that of intermediates generated by wildtype cultures. An enzyme system involved in lignin degradation has been discovered in our Streptomyces. Mutants and recombinants which are enhanced in lignin degrading ability also produce higher levels of this enzyme complex, which catalyzes the cleavage of β-ether linkages in lignin. The studies are aimed at developing an understanding of the pathways and genetics of lignin catabolism in Streptomyces. The application of our research findings will be the development of bioconversions for the production of chemicals from lignin, a renewable underutilized resource. Genetically manipulated strains already show promise for use in bioconversions to produce useful modified lignin polymers.

37. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

FATTY AND AROMATIC ACID CATABOLIZING BACTERIA IN METHANOGENIC ECOSYSTEMS $65,000
Marvin P. Bryant
Department of Dairy Science

The goals of this project are to isolate and describe the biochemical ecology and systematics of syntrophic cocultures of proton-reducing (H_2-forming) acetate-forming bacteria or pure cultures of bacteria that catabolize fatty acids and benzenoids in the complex food web of bacteria degrading organic matter to CO_2 and CH_4. Species PA-1 and P-2 from digester sludge degrade phenylacetate (PA), phenol (P), benzoate and phenylpropionate in coculture with H_2-using *Wolinella* (W) which reduces fumarate to succinate. PA-1 + W produces mainly acetate, propionate, succinate and CO_2 from PA and fumarate and catabolizes many other lowly substituted benzenoids and other compounds not used by W or, so far, by PA-1 alone. P-2 + W produces mainly acetate, succinate and CO_2 from P and fumarate. Two new rumen species catabolize methoxy-benzenoids to hydroxy-benzenoids and produce acetate or butyrate. A third new rumen species catabolizes trihydroxy-benzenoids such as gallate, with equimolar H_2 or formate required, to acetate, butyrate and caproate and catabolizes crotonate but not many other possible energy sources to acetate and butyrate in the presence or absence of formate. *Peptostreptococcus productus* from sludge and intestinal tract of man is shown to be the most rapid CO and H_2-CO_2-using mesophilic acetogen as yet documented. Our theory that syntrophy with H_2-using bacteria is necessary for anaerobic catabolism of saturated fatty acids other than formate and acetate and benzenoids containing less than three hydroxyls on the benzene ring to non-benzenoid products in methanogenic ecosystems is so far supported and little or none of this usually occurs in gastro-intestinal tract methanogenic ecosystems. Biochemical, physiologic and systematics research in these areas is continuing.

38. UNIVERSITY OF ILLINOIS
Urbana, IL 61801

PHOTOSYNTHESIS IN INTACT PLANTS $106,000
A.R. Crofts
Department of Physiology and Biophysics

Information on functional aspects of photosynthesis in intact plants, especially on the operation of electron transfer and energy conversion processes, has been limited by the availability of suitable instrumentation. We are developing several items of apparatus for measuring these reactions on intact plants in the field. The instruments are being developed, and used in *in vivo* studies, in parallel with studies in the laboratory using similar instruments for measurement of reactions *in vitro* with isolated chloroplasts. Two portable instruments have been built, and a third is in development. These measure the kinetics of electron transfer through the two-electron gate (the herbicide binding site) using a double flash technique, fluorescence induction kinetics (continuous illumination), and spectrophotometric changes, respectively. The micro-computer based instruments weigh 10-20 lbs., are battery powered, and completely portable. We have been using the first of these instruments to study the kinetics of reduction of plastoquinone in herbicide-resistant weeds, and have identified a characteristic inhibition of this reaction in all atrazine-resistant biotypes so far studied. *In vitro* studies suggest that this symptom is associated with a change in affinity of the binding site for plastoquinone on PS II, and a much greater change in affinity for the herbicide. Our studies account for the lowered growth-yields of the herbicide-resistant plants in terms of an increase in photochemical "misses" due to the altered equilibrium constant for electron transfer in this reaction. We are extending our studies to the characterization of other environmental effects, and continuing a program of basic research into electron transfer on the donor and acceptor sides of PS II.

39. UNIVERSITY OF ILLINOIS
Urbana, IL 61801

MECHANISM OF PROTON PUMPING IN BACTERIORHODOPSIN $72,618
Thomas G. Ebrey
Department of Physiology and Biophysics

The purple membrane of *Halobacterium halobium* probably represents the simplest biological solar energy conversion system. Light absorbed by bacteriorhodopsin, a small protein whose chromophore is retinal, directly leads to the transport of protons across the cell membrane. The resulting chemiosmotic potential can be used to make ATP. An additional feature of the purple membrane is its ability to pump protons over a wide variety of salt concentrations including in extreme saline environments. This proposal is to investigate the relationship between the transport of protons across the membrane and structure and conformation of bacteriorhodopsin. We have made an especially intriguing discovery, that the number of protons released by purple membrane sheets by light can be drastically altered by the proteolytic removal of a few amino acids from the C-terminal "tail" of bacteriorhodopsin. We have also determined that the number of protons pumped also depends on the presence of the C-terminal tail. Most recently we have discovered that bacteriorhodopsin tightly binds divalent cations and this binding partially depends on the presence of the C-terminal tail. We are continuing to investigate the role of the cations and the tail on proton pumping.

40. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

DEVELOPMENT OF A GENETIC SYSTEM FOR *BACTEROIDES* $50,000
Jeffrey F. Gardner and Abigail A. Salyers
Department of Microbiology

The goal of this project is to develop a method for introducing foreign DNA into *Bacteroides* so that polysaccharide catabolism by these bacteria can be studied at the genetic level. We have constructed several chimeric plasmids which contain DNA from *E. coli* plasmids and DNA from pBF4, the conjugal *Bacteroides* plasmid which codes for clindamycin resistance. We have demonstrated that R751 can mobilize one of these chimeric plasmids, pE52, from *E. coli* to *Bacteroides uniformis* and *Bacteroides thetaiotaomicron*. pE52, which contains only 3.8 kb of pBF4 DNA, is stable in *E. coli* and in *Bacteroides*. By contrast, some of our chimeric plasmids which contain larger segments of pBF4 DNA are highly unstable and participate in genetic rearrangements in *E. coli*. We have preliminary evidence that this may be due to the presence of a transposable element which carries the gene for clindamycin resistance. We are now attempting to demonstrate that there is a transposable element and that it can transpose in *Bacteroides*. If so, we will determine whether it can be used for transposon mutagenesis of *Bacteroides*. In addition to our work on construction of chimeric plasmids we have cloned DNA fragments from *Bacteroides thetaiotaomicron* which appear to carry genes for two polysaccharide-degrading enzymes. We will use these clones to investigate the regulation of the enzymes in *Bacteroides*.

41. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

BIOCHEMICAL AND BIOPHYSICAL STUDIES ON *E.COLI* AEROBIC RESPIRATORY CHAIN $85,000
Robert B. Gennis
Departments of Chemistry and Biochemistry

Bacteria use a mechanism similar to mitochondria and chloroplasts to conserve energy and convert it to a usable chemical from. In particular, a transmembrane "proton motive force" is generated concomitant with electron flow through an electron transport chain. We are studying the components in the *E.coli* membrane responsible for generating this electrochemical gradient. E.coli has been selected because of the relative ease with which genetics can be applied to the problem, and also because of the apprent simplicity of the electron transport chain. We are emphasizing the coordinate application of biochemical, immunological and genetics techniques to identify and characterize each component of the aerobic respiratory chain. Our attention has focussed on the cytochrome *d* terminal oxidase complex which we have recently purified and reconstituted in an artifical, energy-conserving liposome system. Our attentions will now focus on the cytochrome *o* complex, about which much less is known. We have immunologically characterized this and demonstrated that it contains two *b* cytochromes, 4 polypeptide subunits, and functions as a "coupling site" or point of proton translocation in the membrane. The enzyme has also recently been purified to homogeneity and mutant strains lacking this enzyme have been isolated. The combined use of genetics and biochemical characterization will result in a detailed understanding of this system in the near future.

42. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

GENETICS OF THE METHANOGENIC BACTERIUM, *METHANOCOCCUS VOLTAE* WITH ATTENTION TO GENETIC CONTROL MECHANISMS $50,000
Jordan Konisky
Department of Microbiology

The objectives of this project are to both develop a genetic system and to characterize gene expression in the methanogen, *Methanococcus voltae*. We have previously reported the cloning of methanogen arginine and histidine biosynthetic genes. These genes are being characterized with particular emphasis on the elucidation of promoter and other DNA sequences involved in the regulation of gene expression. We are also investigating the molecular basis of our finding that methanogen genes which are expressed weakly in *E. coli* can be activated by the insertion of *E. coli* DNA into methanogen sequences. Controlled methods are being developed for the isolation of methanogen mutants which are resistant to antibiotics and other agents which inhibit methanogen growth. Such mutants will be examined in an attempt to define the molecular basis for such resistance. These studies serve as a useful approach to probe methanogen metabolism and surface structure. In an attempt to develop gene vectors for gene transfer into methanogens, we are screening new *Methanococcus* isolates for the presence of plasmids. Such plasmids would be engineered to contain appropriate genes for selection of transferred DNA. This approach complements other attempts to develop a gene transfer system such as direct transformation of protoplasts or protoplast fusion.

43. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

THE ROLES PLAYED BY MITOCHONDRIAL DNA PLASMIDS AND NUCLEAR GENES IN REVERSIONS TO FERTILITY IN S-TYPE MALE-STERILE MAIZE — $80,810
John R. Laughnan
Department of Genetics and Development

These investigations involve coordinated field and laboratory studies on cytoplasmic male sterility (CMS) in maize, with principal focus on genetic changes in nuclear and mitochondrial DNA (mtDNA) that accompany reversions from CMS to male fertility at both the nuclear and cytoplasmic levels. They also aim at a better understanding of the organization of the main mitochondrial chromosome and of so-called satellite DNA molecules that co-exist as plasmid like elements in the mitochondrion. A first approach involves studies at the molecular level on nuclear reversion to male fertility and will employ maize transposable controlling elements to identify nuclear restorer genes at different chromosomal sites, and to isolate and characterize them at the molecular level. We are also investigating the molecular characteristics of a variety of cytoplasmic male fertile revertents; major characteristics of these revertents appear to be determined by the nuclear genotype. We are extending the studies indicating that plasmid disappearance upon cytoplasmic reversion is dependent on nuclear genotype and are also investigating whether the overall organization of the mitochondrial genome is governed by nuclear genotype, as preliminary results suggest. Developmental aspects of the event will be studied further; it is now possible to relate left and right halves of the tassle to corresponding halves of the stem and leaf portions of the plant, and therefore to correlate ear performance with the positions of tassle reversion events. Recent genetic studies indicate that the nuclear restorer elements of CMS are transposable, and further studies are now under way to determine how this behavior correlates with that of the known controlling elements in maize, and to identify special characteristics of the transposition event in this case.

44. UNIVERSITY OF ILLINOIS
Urbana, Illinois 61801

ACETOCLASTIC METHANOGENESIS — $70,777
Ralph S. Wolfe
Department of Microbiology

We propose to define the enzymology of methane formation from acetate by aetophilic methanogens. Knowledge of the biochemistry of this area of methanogenesis lags far behind that of methanogenesis from CO_2 and H_2 largely because of the difficulty in mass culturing cells on acetate. However, in nature about 70% of the methane formed is derived from the methyl group of acetate, an indication of the importance of this process in anaerobic biodegradation. We propose to follow the strategy that we have used successfully to study the biochemistry of methanogenesis in other methanogens. This involves mass culture of the organism, development of a fractionation procedure to resolve the enzymes and coenzymes, development of procedures for purification of the components to the homogeneous state, and definition of the role of each component. These basic studies are prerequisite to an understanding of the acetophilic methanogens and their role in anaerobic degradation.

45. THE INSTITUTE OF PAPER CHEMISTRY
Appleton, Wisconsin 54912

RAMAN MICROPROBE INVESTIGATION OF MOLECULAR STRUCTURE AND ORGANIZATION IN THE NATIVE STATE OF WOODY TISSUE $46,340

Rajai H. Atalla
Chemical Sciences Division

The objective of this project is to explore molecular structure and organization in the cell walls of native woody tissue. The primary investigative tool is the Raman microprobe which has made possible spectroscopic exploration of domains of the order of 1 μm in sections of native tissue. Preliminary explorations on tissues from loblolly pine (*Pinus taeda* L) and from black spruce (*Picea mariana*) revealed evidence of variations in composition within the secondary walls of individual cells as well as between adjacent cells in the same annual ring. They also provided indications of molecular orientation relative to the plane of the cell walls. More recent studies focussing on tissue from *Picea mariana* have shown that, in a majority of locations in the secondary wall, the phenyl propane units of lignin are preferentially oriented in the plane of the cell wall. The spectral features associated with cellulose are consistent with alignment of the anhydroglucose rings perpendicular to the plane of the cell cross section. The continuing effort is directed at a mapping of the patterns of variation of both composition and molecular orientation. The results further our fundamental understanding of cell wall architecture and can be of use in analysis and design of industrial processes which use biomass as a primary resource.

46. IOWA STATE UNIVERSITY
Ames, Iowa 50011

PROLINE METABOLISM IN PLANTS UNDER ENVIRONMENTAL STRESSES $62,000

Cecil R. Stewart
Department of Botany

The goal of this project is to understand the subcellular mechanism which causes proline to accumulate under environmental stresses. Since one of the known causes is inhibition of proline oxidation, we have continued our studies of this process in mitochondria. Mitochondrial proline transport has been measured by osmotically induced size changes in combination with oxygen uptake. Uptake is absolutely stereospecific and partially dependent on the energy of an electrochemical gradient. Based on the effects of FCCP and valinomycin, it has been shown that uptake is gradient dependent only at high proline concentrations and it is the pH component of the gradient that drives uptake rather than the electrical component.

Steady state proline levels in stressed leaves have been determined to find the relationship between proline levels and salt content. A linear relationship between salt and proline content above a threshold salt level is consistent with proline functioning as a compatible osmoticum and excess salt being accumulated in the vacuole. Changes in proline levels during recovery from wilting have been contrasted with changes after removal from salt and are consistent with proline levels responding to reversible changes in salt concentration during dehydration and rehydration. Current studies are aimed at testing these interpretations directly using isolated protoplasts and vacuoles.

These results contribute to our understanding of plant adaptions at the molecular level and provide information on which to base possible plant manipulations using new molecular techniques.

47. UNIVERSITY OF KENTUCKY
Lexington, Kentucky 40546-0091

PHYSIOLOGY/BIOCHEMISTRY OF PHOTOACTIVATION OF OXYGEN EVOLUTION: PROBES FOR THE S-STATE PROTEIN $28,328 (FY 83)
George M. Cheniae
Agronomy Department

This project is focused towards: 1) elucidation of the biochemical/physiological reactions underlying the multiquantum process required for the photoactivation of O_2 evolving centers; and 2) studies of the multimeric O_2 evolving center (OEC) with emphasis on the subunit compositional effects on O_2 evolution and the reactivity of the topography of the OEC complex to chemical analogs of the H_2O molecule. A number of different studies (developmental; recovery from inactivation of active OEC by heat/cold stress and chemical analogs (NH_2OH) of water) indicate that the photoconversion of inactive OEC to active OEC by PSII during photoactivation is a fundamental process in the oxygenic photosynthetic organisms. We study the photoconversion of inactive to active OEC under two conditions: 1) following a photoinhibition of PSII, which saturates at weak light intensity ($t_{1/2}$~2-3min) and thereby confers requirement for light dependent synthesis of two specific PSII polypeptides on chloroplast 70S ribosomes for reappearance of active OEC; and 2) photoactivation *per se*, a process independent of protein synthesis, in which Mn^{+2} and specific PSII polypeptides of the OEC complex are assembled into thylakoids to yield active OEC centers. The other focus of this project involves selective extraction of subunits of the OEC, subsequent reconstitutions and determination of effects on O_2 evolution, PSII reactions, and modifications of reactivity of OEC to chemical analogs of H_2O. These studies include effects of specific protein-modifying reagents and specific affinity/photoaffinity reagents containing groups known to react rather specifically with OEC.

48. LEHIGH UNIVERSITY
Bethlehem, Pennsylvania 18015

A GENETIC APPROACH TO SECRETION AND HYPERPRODUCTION OF CELLULASE BY *TRICHODERMA* $82,900
Bland S. Montenecourt and Jeffrey A. Sands
Department of Biology and the Biotechnology Research Center

Cellulases are important glycoprotein enzymes of great potential industrial importance in the recycle and use of cellulosic biomass. Production of cellulases by fungi involves protein synthesis at the level of the endoplasmic reticulum, glycosylation in the endoplasmic reticulum and presumably the Golgi complex followed by packaging into secretory vesicles and finally secretion to the external milieu. Little is known of the precise sequence of events involved in the production of extracellular glycoprotein enzymes by lower eukaryotic microorganisms. In an effort to elucidate these steps, we are employing the cellulase system of *Trichoderma reesei* as a model. We have isolated a range of auxotrophic, drug resistant and temperature sensitive mutants from both the wild type, QM6a, and a number of the high yielding cellulase mutants which we have previously isolated (e.g., RL-37 and Rut-C30). We are developing a recombination system by heterokaryon formation and protoplast fusion to identify the various steps in secretion. In addition, we are studying the effects of glycosylation inhibitors and membrane perturbing agents on the biochemical nature of the enzymes and the secretory pathway. A better understanding of cellulase biosynthesis at the molecular level should result in more selective and sensitive systems for isolating improved mutants and contribute toward fermentation optimization.

49. **MARTIN MARIETTA LABORATORIES**
1450 South Rolling Road
Baltimore, Maryland 21227-3898

STUDIES OF PHOTOSYSTEM II USING ARTIFICIAL DONORS — $95,370
Dr. Richard Radmer
Biosciences Department

The goal of this project is to study aspects of photosynthetic oxygen evolution using specialized mass spectrometric and spectrophotometric techniques. We are using a mass spectrometer system constructed in-house to monitor the amount and isotopic composition of the gas exchange elicited by short saturating flashes, e.g., O_2, N_2 from NH_2OH oxidation, $^{18}O_2$ from $H_2{}^{18}O$ oxidation, etc. Studies using $H_2{}^{18}O$ are being carried out to determine whether there are bound non-exchangeable (partially oxidized?) intermediates generated during the course of H_2O oxidation to O_2. We are also using "H_2O analogs," i.e., hydroxylamine and hydrazine and their methyl-substituted derivatives, to attempt to characterize various modified TSF2 System-II preparations. (These studies are based on our earlier work using broken chloroplasts.) A spectrophotometric TMPD assay, developed earlier in our laboratory, is being used to ascertain the population of active and inactive O_2-evolving centers in a given preparation. The aim of these studies is to correlate the topography of the O_2-evolving site (as determined by the reactions of the H_2O analogs) with the protein complement and the photochemical activity of the modified TSF2 preparations.

50. UNIVERSITY OF MARYLAND
College Park, Maryland 20742

ENERGY-DEPENDENT CALCIUM TRANSPORT MECHANISMS IN PLANT MEMBRANES — $63,558
Heven Sze
Department of Botany

The objectives of this project are (i) to identify and characterize active calcium (Ca) transport systems in higher plant tissues and (ii) to understand the mechanisms that regulate Ca fluxes. Plant tissues include tobacco callus (*Nicotiana tabacum*), oat (*Avena sativa*) and corn (*Zea mays*) roots. Subcellular membranes are isolated and purified by differential and density centrifugation, and ATP-dependent 45-Ca uptake is measured by a filtration procedure. At least two types of ATP-dependent Ca transport systems have been identified in microsomal vesicles using specific inhibitors and ionophores: one requires a pH gradient and one does not. The Ca/H antiport is anion-sensitive and vanadate-resistant suggesting that Ca uptake is driven by a pH gradient generated by a tonoplast-type H-pumping ATPase. Another Ca pump (probably a Ca-pumping ATPase) is vanadate-sensitive and experiments are underway to determine the membrane identity. To understand how Ca fluxes are regulated, the effect of phytohormones and toxins on the various Ca transport systems will be studied. For example, we have found that a fungal toxin (*Helminthosporium maydis* T) decreases active Ca transport into isolated mitochondria from susceptible corn but not resistant corn. We are conducting studies to determine more specifically the mode of toxin action. Since Ca levels are important in regulating various physiological and biochemical processes, these studies of Ca transport are central to our understanding of not only the mechanism and regulation of solute transport but also the regulation of plant growth and development.

51. **MASSACHUSETTS INSTITUTE OF TECHNOLOGY**
Cambridge, Massachusetts 02139

ANTIBODY ANALYSIS OF THE RHIZOBIUM MELILOTI SURFACE $80,000
Ethan R. Signer
Department of Biology

Rhizobium meliloti forms nitrogen-fixing nodules on the roots of alfalfa. Both polyclonal sera and monoclonal antibodies (MAb) to the bacterial surface will be used to identify components essential for the initial nodulation step(s). Immunoprecipitation analysis with polyclonal sera will be used to identify components differing in isogenic Nod$^+$ and Nod$^-$ pairs. MAb will be produced and used to isolate Ab-insensitive nodulation-defective (Nod$^-$) mutants by methods we have developed. Surface changes as a function of growth conditions and phases will be studied. Several methods will be tried to circumvent immunodominant antigens and reveal weaker ones, particular immunosuppression in combination with in vitro immunization. Two defects in later nodulation stages identified in earlier work will also be pursued.

52. UNIVERSITY OF MASSACHUSETTS
Amherst, Massachusetts 01003

CONVERSION OF CELLULOSE TO ETHANOL BY MESOPHILIC BACTERIA $77,000
Ercole Canale-Parola, Clifton E. Dowell, and
Susan B. Leschine
Department of Microbiology

The main objective of the project is to study the genetics of mesophilic anaerobic bacteria that ferment cellulose to ethanol. The bacteria used in this investigation are strains of Clostridium that i) convert to ethanol not only cellulose, but also components of the hemicellulosic portion of biomass, and ii) are relatively ethanol tolerant. The studies include plasmid analysis, as well as fine-structure mapping of genes involved in the breakdown of cellulose to soluble sugars. These genes code for cellulase system enzymes such as endo-1,4-β-glucanases, exo-1,4-β-glucanases, β-glucosidases, and cellobiose phosphorylase. The research includes characterization of cellulase system enzymes present in ethanol-producing mesophilic clostridia, as well as of enzymes utilized by these bacteria in the breakdown of hemicellulosic components. The work will provide fundamental information on the genetics of cellulose-fermenting, ethanol-producing clostridia. This information will be valuable for the understanding of metabolic processes utilized by anaerobic bacteria to degrade cellulose, and for the development of clostridial strains that can be used in the industrial conversion of biomass to ethanol. Finally, the research will elucidate basic aspects of the genetics of clostridia. At present, very little is known about the genetic systems of this large group of anaerobic bacteria.

53. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824-1312

CONTROLLED MEDIA FOR PLANT TISSUE CULTURE
Norman E. Good
Department of Botany and Plant Pathology

$55,000
(FY 83)

We are very disturbed by the fact that commonly used plant tissue culture media are uncontrolled, with constantly changing levels of hormones, vitamins, nutrients and pH. Consequently, we are exploring ways of stabilizing most of these factors. The techniques used are: 1) To buffer substances by having a reservoir of bound substance in equilibrium with the free solution. Thus we are exploring the use of H^+ buffers to regulate pH and the use of charcoal or ion-exchange resins pre-equilibrated with hormones and vitamins to maintain their concentrations; 2) To provide reservoirs in the form of conjugates of hormones which are in themselves metabolically inactive but break down slowly to give reasonably constant levels of the free active form of the substance. This technique is especially useful for maintaining a variety of constant auxin levels, the level depending on which conjugate is used; 3) To provide hormones which are chemically and metabolically stable, for instance the auxin analogue 2,4-D. This approach has been used widely but at a great penalty since by so doing one tends to frustrate any attempt by the tissue to regulate messages being sent, the same hormonal message being read over and over, probably at the cost of differentiation. Using these techniques we are looking again at recalcitrant tissue culture systems, where there have been problems of producing or maintaining callus from organized tissue, of inducing the development of callus from protoplasts, and of inducing organogenesis from callus.

54. UNIVERSITY OF MINNESOTA
St. Paul, Minnesota 55108

CORN STORAGE PROTEIN - A MOLECULAR GENETIC MODEL
Joachim Messing
Department of Biochemistry

$103,950

The current work is an extensive study of the nucleotide sequences of the genes in maize encoding the most abundant class of storage proteins in the endosperm tissue, the zein protein family. These studies emphasize the use of a recently developed tool in recombinant DNA technology, the M13 cloning system to produce the data and the aid of a computer in analyzing the data. We assume that the efforts in improving the methodology of the M13 system are justified because of their impact on research of gene structure and function in many laboratories. We have used these techniques to study differential gene expression in an economically important plant, corn. To understand the control mechanism of gene expression during tissue development, we have chosen the zein multigene family as a molecular genetic model. These genes represent a particularly interesting case because zein proteins accumulate in large quantities, are synthesized exclusively in the endosperm tissue, consist of a large closely related family of proteins, and are synthesized during a brief period of development. They make up to 50% - 60% of the total protein in the corn kernel (Nelson, 1969) and, therefore, represent a major component in the feed of livestock. Ultimately, the physical basis of the control of the expression of these genes much reside in their nucleotide sequence.

55. UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota 55455

THE MECHANISM OF SWITCHING FROM AN ACIDOGENIC TO A BUTANOL-ACETONE FERMENTATION BY *CLOSTRIDIUM ACETOBUTYLICUM* $74,000
Palmer Rogers
Department of Microbiology, Medical School

The obligate anaerobic bacteria, *Clostridium acetobutylicum*, ferments sugars to form acetic and butyric acids during early growth and then later produces entirely ethanol, acetone, and butanol. Experiments are designed to investigate the molecular mechanisms used by this bacteria to regulate the shifting of the enzyme activities catalyzing the four-branched fermentation pathways.

Following mutagenesis with N-nitrosoguanidine or ethylmethane sulfonate, we are screening for three different classes of mutants. Initially we have isolated rifampicin-resistant and streptomycin-resistant mutants as a rapid screen for the development of protoplast fusion. Secondly, amino acid auxotrophs will be selected, since these bacteria grow slowly without amino acids in the presence of vitamins. Thirdly, using plates with indicator dyes, fermentation mutants producing limited acid or limited alcohols will be isolated.

Protoplast fusion of *Clostridium acetobutylicum* is under study. Protoplast formation and regeneration techniques are now combined with protoplast fusion methods to produce double-mutants from single drug resistant parents. Protoplast fusion will be used in conjunction with a panel of acid-non-producer mutants to determine the number of factors regulating the fermentation program of this bacteria.

Enzyme activities were monitored from cell-free extracts for butanol and butyric acid formation. We find a rapid 100 fold rise in butanol forming enzymes coordinate with production of butanol followed by a rapid decay of activity when butanol synthesis stops. Experiments are designed to determine the role of enzyme synthesis and activity modification during these changes.

56. UNIVERSITY OF MINNESOTA
St. Paul, Minnesota 55108

MOLECULAR APPROACHES TO GENOMIC ORGANIZATION $58,780
Irwin Rubenstein
Department of Genetics and Cell Biology
Ronald L. Phillips
Department of Agronomy and Plant Genetics

We propose to develop physical methods to determine the chromosomal location of isolated maize genomic segments. The first procedure uses a modified dot hybridization technique combined with the use of DNAs from a series of trisomic, disomic and monosomic maize plants. We have been able to demonstrate (in simulation experiments) the capacity to distinguish the presence of one versus two copies of unique genomic segments. This experiment is now being repeated with a number of genomic probes. The second procedure uses ^{3}H or ^{125}I-labeled RNA probes for *in situ* hybridization to determine the chromosomal location of genomic segments present at low reiteration frequencies. Highly labeled probes have been produced from genomic clones transferred to a transcription vector that contains a bacteriophage SP6-specific RNA polymerase promoter. These RNA probes give a high detection sensitivity and a low grain background.

57. UNIVERSITY OF MISSOURI
Columbia, MO 65211

PHOTOSYNTHESIS, CLONING, AND BIOCONVERSION OF SOLAR ENERGY IN CYANOBACTERIA $66,764
Louis A. Sherman
Division of Biological Sciences

The goal of this proposal is to identify and clone the genes coding for membrane proteins involved in cyanobacterial photosynthesis. Cyanobacteria represent an excellent organism for such studies since they perform an aerobic photosynthesis nearly identical to green plants, and they are suitable for genetic, biochemical, and biophysical studies in photosynthesis. The organisms used for these studies, *Anacystis nidulans* R2 and *Aphanocapsa* 6714, are both transformable strains, and can thus be used for experiments involving genetic manipulation. We are using three types of experimentation to identify and clone specific genes. The first procedure utilizes heterologous probes to detect and clone related genes from *A. nidulans*. This procedure has enabled us to clone the genes coding for a Ca^{+2}-binding protein homologous to calmodulin, the rapidly-turned over, 32kDa, atrazine-binding protein (and the gene from a DCMU-resistant mutant that gives rise to the resistant-phenotype), the P700 Chl a-binding protein, and subunit IV of the cytochrome b$_6$/f complex. We have also isolated DCMU and Cd-resistant mutants in *A. nidulans*, characterized the specific lesion, and used the transformation system to isolate the appropriate gene. Interesting, both mutants appear to affect (at least in part) the same PSII protein; this is a 34kDa species that is also rapidly-turned over. In the DCMU-resistant mutant, the protein is altered to a 35.5 kDa polypeptide, whereas in the Cd-resistant mutant the turnover appears to be affected. The Cd-resistant mutant demonstrates a low fluorescence phenotype, implying that the 34kDa protein functions on the oxidizing side of PSII. Finally, we are using transposon mutagenesis in the heterotrophic strain *Aphanocapsa* 6714. This technique will generate mutants affecting oxygen-evolution and PSII activity; we will then use the antibiotic marker on the transposon to clone the specific genes.

58. MOUNT SINAI SCHOOL OF MEDICINE OF CUNY
New York, New York 10029

THE RESPIRATORY CHAIN OF ALKALOPHILIC BACTERIA $72,828
Terry Ann Krulwich
Department of Biochemistry

Obligately alkalophilic bacteria contain extraordinarily high concentrations of membrane-bound respiratory chain components and an apparently complex respiratory chain, with many redox carriers distinguishable by their midpoint potentials. It has been proposed that the alkalophile respiratory chain possesses structural/functional properties, of which the complexity is a part, which facilitate particularly effective energy conservation. This, in turn, helps meet the special energy costs of life at very high pH. Initial studies of H$^+$ translocation support this hypothesis. More detailed studies of H$^+$ translocation will be conducted using whole cells, protoplasts and/or vesicles, and reconstituted systems. The characteristics of the respiratory chain complex III and cytochrome oxidase will be examined further, the latter complex has been purified to homogeneity from *Bacillus firmus* RAB. The regulation of cytochrome levels and arrays are of particular interest in this system because of the observation that non-alkalophilic mutants have quantitatively and qualitatively fewer cytochrome species. Protocols for study of cytochrome expression, as a function of pH, have been developed.

59. NATIONAL INSTITUTE OF GENERAL MEDICAL SCIENCES
National Institutes of Health
Bethesda, Maryland 20205

GENBANK (TM), THE GENETIC SEQUENCE DATA BANK — $40,000
Christine K. Carrico

GenBank(tm), the Genetic Sequence Data Bank, is an internationally available repository of all reported nucleotide sequences greater than fifty nucleotides in length, annotated for sites of biological interest and checked for accuracy. As of April 1, 1984, GenBank contained 2.94 million bases, comprising 3576 sequences. The data bank is operated under contract to Bolt Beranek and Newman Inc. (BBN) of Cambridge, MA. Data collection, verification, entry and annotation are performed under the direction of Dr. Walter Goad at Los Alamos National Laboratory, while distribution, user support services and overall data bank management are performed by BBN. This resource, co-sponsored by the National Institute of General Medical Sciences, National Cancer Institute, National Institute of Allergy and Infectious Diseases, National Institute of Arthritis, Diabetes, Digestive and Kidney Diseases, and Division of Research Resources (of NIH), the National Science Foundation, the Department of Energy and the Department of Defense, is of particular interest to geneticists and molecular biologists. A copy of the database is available for a modest fee on computer-readable magnetic tape to anyone requesting it. Dial-up on-line access, including Telenet access, is also available to anyone, but only a limited number of users can be accommodated at any one time. The first hard-copy edition of the database was available in May 1984 as a 2-volume supplement to *Nucleic Acids Research* and contained the combined databases of GenBank and the European Molecular Biology Laboratory's Nucleotide Sequence Library. Curators have been appointed to oversee selected portions of the database and more are to be appointed this year. Work is currently in progress to provide GenBank users with a directory of information about the availability of sequence analysis and manipulation software that can be used with GenBank.

60. UNIVERSITY OF NEBRASKA-LINCOLN
Lincoln, Nebraska 68583-0718

BIOCHEMICAL AND PHYSIOLOGICAL CHARACTERIZATION OF HIGHER PLANTS WITH REDUCED PHOTORESPIRATION — $40,000
Raymond Chollet
Department of Agricultural Biochemistry

The ultimate goal of this project is to elucidate mechanisms which reduce photorespiration and the associated O_2 inhibition of photosynthesis in terrestrial higher plants. Only two such mechanisms for reducing this seemingly wasteful metabolic process are known in nature, both of which involve a biochemical CO_2-concentrating system to provide the bifunctional enzyme ribulosebisphosphate carboxylase/oxygenase (RuBisCO) with an elevated pCO_2/pO_2 ratio. However, recent findings in this laboratory [Holaday & Chollet (1983) Plant Physiol. 73:740-745] and elsewhere indicate that neither of these two known mechanisms is operative in *Moricandia arvensis* and *Panicum milioides*. Yet, it is firmly established that bundle-sheath ultrastructure and photorespiratory activity in intact leaves of both species are intermediate between those features of C_3 and C_4 plants [Holaday et al. (1981) Biochim. Biophys. Acta 637: 334-341, (1982) Plant Sci. Lett. 27: 181-189]. Present studies indicate that: (i) the RuBisCO enzyme is neither altered kinetically [CO_2/O_2 specificity factor, Km(CO_2)] nor compartmented intercellularly between the mesophyll and bundle-sheath chloroplasts in both C_3-C_4 intermediate species; and (ii) *M. arvensis* and *P. milioides* may reduce photorespiration, at least in part, by internally refixing photorespiratory CO_2 via RuBisCO more efficiently than closely related C_3 species (*M. foetida*, *P. laxum*). Future investigations will pursue this latter aspect in greater detail with isolated leaf cell-types and organelles and evaluate whether the recently discovered C_3-C_4 intermediate *Flaveria* species [Holaday et al. (1984) Planta 160: 25-32] possess a limited C_4-like CO_2-concentrating system or some other mechanism(s) for reducing photorespiration.

61. UNIVERSITY OF NEBRASKA
Lincoln, Nebraska 68583-0722

VIRUSES OF EUKARYOTIC GREEN ALGAE — $65,000
James L. Van Etten
Department of Plant Pathology

We have recently isolated and partially characterized four distinct dsDNA viruses which replicate in *Chlorella*-like green algae symbiotic with *Hydra* and *Paramecium*. One of these viruses, PBCV-1, also synchronously infects and replicates in two culturable *Chlorella*. This has allowed, for the first time, the production of mg quantities of a eukaryotic algal virus as well as the development of a plaque assay for PBCV-1. The PBCV-1 *Chlorella* system is the first example of a virus infecting any eukaryotic plant which can utilize procedures directly adapted from those used to study bacteriophage.

The objective of this proposal is to determine the structural organization and properties of the large viral genome (ca. 300 kbp) and the nature and function of the viral gene products. The research has several potentially important long range implications. Studies on PBCV-1 will: (i) provide an opportunity to study a new type of virus-host relationship, (ii) determine the role it plays in symbiosis, (iii) demonstrate the usefulness of PBCV-1 or PBCV-1 DNA as a vector for transferring genes into other algae or higher plants, and (iv) determine if PBCV-1 or PBCV-1 lysates contain a new source of plant cell wall degrading enzymes. Finally studies on the regulation and expression of the dsDNA viral genome in the host will provide new information on gene regulation in eukaryotic plants.

62. NEW YORK STATE DEPARTMENT OF HEALTH
Center for Laboratories and Research
Albany, New York 12201

METHANE PRODUCING BACTERIA: IMMUNOLOGICAL CHARACTERIZATION — $55,000
Conway de Macario, E.,[*] Macario, A.J.L.,[*] and Wolin, M.J.[•]
[*]Laboratory of Immunology
[•]Laboratory of Environmental Biology and Field Services

The long-term goals of this research is to standardize methods for immunologic examination of microbial communities containing methanogens and to determine the antigenic fingerprint of these bacteria. Procedures for sampling microbial communities of practical importance, e.g. digesters, are being developed to obtain specimens amenable to serologic analysis. The antigenic fingerprints of methanogens in these specimens are being determined at various time intervals. The presence of antigenic markers of methanogens in the fluid phase is also being investigated, not only in digesters, but also in bacterial cultures and suspensions of various kinds. Specific objectives are to develop methods for rapid, direct identification of "serotypes" by assaying the bacteria themselves and/or their markers released into the fluid phase, and to monitor the methanogenic population during operation of digesters. Correlations serotype(s)/digester's performance are being sought for. These studies should yield new methodology applicable to the analysis of a variety of complex ecosystems, and should help improve biotechnology concerned with elimination of organic wastes and production of methane. The methods and the data should also be useful in genetic engineering involving methanogens.

63. STATE UNIVERSITY OF NEW YORK AT BINGHAMTON
Binghamton, New York 13901

GENE-ENZYME RELATIONSHIPS IN SOMATIC CELLS AND THEIR ORGANISMAL DERIVATIVES IN HIGHER PLANTS — $90,000
Roy A. Jensen
Center for Somatic-cell Genetics and Biochemistry

Our long-term objectives are to establish in a higher plant an experimental system that is firmly defined by biochemical, genetic, and physiological criteria. Since somatic cells can be cultured essentially as microbial populations, even to the extent of obtaining recessive mutations that can be expressed in haploid cells, the ability of appropriately manipulated cells to regenerate to the organismal state allows exceptional opportunities to study development. *Nicotiana silvestris* and/or *N. plumbaginifolia* are the organisms of choice, and the pathway of aromatic amino acid biosynthesis is the focal point for study of gene-enzyme relationships. Highlights of our multiphasic approach are the identification and characterization of the biochemical steps associated with the synthesis of aromatic amino acids, the subcellular partitioning of these enzymes between different intracellular compartments, and the characterization of key regulatory enzymes. We will isolate both regulatory mutants and structural-gene mutants, and will seek to regenerate plant organisms which express such mutations. Completion of the latter objective may require temperature-sensitive mutations. Molecular-genetic approaches will be taken to identify and isolate genes, to use them as probes to study gene expression, and to establish gene locations. We seek to understand physiological, biochemical, developmental, and genetic interrelationships that are associated with an important biosynthetic pathway in a single experimental system. The aromatic amino acid pathway is of central importance in plant metabolism. Analysis of this pathway could have profound impact on the understanding of the biology of the plant because the pathway leads to protein precursors, growth regulators, a diverse range of secondary metabolites, and to medically significant drugs.

64. UNIVERSITY OF NORTH CAROLINA
Chapel Hill, North Carolina 27514

CHARACTERIZATION OF *TRICHODERMA REESEI* CELLULASE GENES — $87,000
Darrel W. Stafford
Department of Biology

Our laboratory is interested in the structure function relationships of the two major cellobiohydrolases of *Trichoderma reesei*. One of the goals is to achieve expression of high levels of these proteins in *E. coli* and in a fungal system. Questions about the relative activities of glyscosylated vs non glycosylated and mutant proteins will be examined. To this end we have cloned cellobiohydrolase I and cellobiohydrolase II into *E. coli*. The gene for cellobiohydrolase I was identified by synthetic oligonucleotides and shown to be correct by sequence analysis. The gene for CBH II was identified by screening an expression library with an antibody provided by Dr. Ross Brown and Dr. M. Gritzaldi. At present we are still characterizing both clones by sequence analysis.

65. NORTHWESTERN UNIVERSITY
Evanston, Illinois 60201

GENETICS OF THERMOPHILIC BACTERIA

$60,104

Neil E. Welker
Department of Biochemistry, Molecular Biology
and Cell Biology

The goal of this project is to develop reliable genetic exchange systems in thermophilic bacilli. We have demonstrated chromosomal and plasmid DNA transformation in competent cells, transfection with thermophilic phage TP-19, TP-25 and TP-36 DNA, and PEG-induced plasmid DNA transformation of protoplasts in several prototrophic strains of thermophilic bacilli. This group is composed of strains of Bacillus stearothermophilus, Bacillus coagulans, Bacillus licheniformis, Bacillus sphaericus, and Bacillus subtilis. The temperature range of growth of these strains overlaps in a continuous manner between 20°C and 90°C. We will determine optimal conditions for preparing competent cells and the regeneration of protoplasts of each strain. Plasmids will be isolated or constructed that are stably maintained in each of these strains. We intend to construct a shuttle plasmid(s) that can be transferred between strains whose combined temperature ranges for growth can be as great as 70 degreees. These techniques will facilitate genetic analysis of thermophilic bacilli; detect intraspecific transfer of genetic information; and clone desired genetic trails (e.g. cellulose hydolysis, ethanol production) from other thermophiles which lack a genetic exchange system and/or possess growth characteristics which make them unsuitable for research. Insights gained from studies with thermophilic bacilli may be used to devise genetic exchange systems in other thermophilic bacteria.

66. OHIO STATE UNIVERSITY
Columbus, Ohio 43210

DEVELOPMENT OF GENETIC SYSTEMS FOR ANALYSIS OF THE OBLIGATE ANAEROBE METHANOBACTERIUM RUMINATIUM PS

$67,000

John N. Reeve and James I. Frea
Department of Microbiology

The goal of this project is to develop techniques which will facilitate genetic analyses of methane producing micro-organisms. We are using a variety of mutagens to isolate drug resistant and auxotrophic mutants of Methanococcus vannielli. A plasmid, pME2001, isolated form Methanobacterium thermoautotrophicum is being used to construct shuttle vectors. Plasmids capable of replication in the methanogen and in Escherichia coli, Bacillus subtilis and/or Saccharomyces cerevisiae are now available. A number of genes capable of complementing auxotrophic mutations of E. coli and, in one case (argA) also a B. subtilis mutation, have been cloned from methanogenic species. These genes are being incorporated into the shuttle vectors to provide selectable traits. Several of the cloned genes are being sequenced. The complete DNA sequences of a gene, isolated from Methanobrevibacter smithii, which complements E. coli proC mutations has been determined. Regions of DNA used to initiate and terminate transcription of this gene, in both E. coli and M. smithii, will be characterized. An insertion sequence which originated in M. smithii (ISM1) has been isolated and sequenced. We are determining the extent to which this element transposes in M. smithii. The insertion sequence will be modified by in vitro enzymatic procedures to create an element capable of introducing DNA into the genome of methanogens. Transformation procedures which are currently used to introduce DNA into bacterial species are being tested, under anaerobic conditions, with M. vannielli to determine if transformation of this species can be obtained using standardized protocols. Shuttle vector DNAs are used as donor DNAs. Successful transformation will be detected by DNA:DNA hybridization using nick-translated plasmid DNAs as the radioactive probes.

67. UNIVERSITY OF OKLAHOMA
Norman, OK 73019

METABOLISM OF FATTY ACIDS BY SYNTROPHOMONAS WOLFEI $47,011
Michael J. McInerney
Department of Botany and Microbiology

The degradation of fatty acids is often the rate-limiting step in the conversion of organic matter to methane and carbon dioxide. Recently, a new metabolic group of bacteria called the hydrogen-producing acetogenic bacteria has been discovered that anaerobically degrades fatty acids with hydrogen production. The slow growth rate of these bacteria and the fact that they can only grow in coculture with hydrogen-using bacteria is a hindrance to the further physiological characterization of this important group of bacteria.
We have developed methods to grow 10-liter batches of *Syntrophomonas wolfei* - *Methanospirillum hungatei* coculture. About 1.5 grams wet weight of cells of the coculture is obtained within 2 weeks. Cell-free extracts of *S. wolfei* are obtained by selectively lysing the *S. wolfei* cells with lysozyme-ethylene diamine tetraacetate and by removing the unlyzed methanogen cells by centrifugation. Quantitation of Factor-420 (a cofactor unique to methanogens) shows that about 98 percent of this material is removed by centrifugation. This indicates that the cell-free extracts of *S. wolfei* are essentially free of contamination by cellular components of the methanogen. High amounts of activity of 3-hydroxyacyl-CoA dehydrogenase were detected in *S. wolfei* extracts. Thus, this procedure yields extracts that are active and essentially free from contamination by cellular components of the methanogen. The methods will be used to study the metabolism and physiology of *S. wolfei*. Particular emphasis will be placed on the mechanisms of energy conservation and hydrogen production.

68. PENNSYLVANIA STATE UNIVERSITY
University Park, Pennsylvania 16802

THE ROLE OF TURGOR PRESSURE IN PLANT GROWTH $61,841
Daniel Cosgrove
Department of Biology

This project is investigating the dependence of plant growth on cell turgor pressure, especially as influenced by conditions of water stress. The growth of pea stems is being measured using marking techniques and high-resolution position transducers. Pea seedlings (*Pisum sativum* L.) are grown under various regimes of water stress. As less water is available to the plant, stem elongation is reduced. We are measuring each of the parameters governing cell growth to elucidate the relationships between water availability, cell turgor pressure and cell growth. Turgor pressure (hydrostatic pressure) in individual cells is directly measured with the micro-pressure probe, a device which also enables us to measure the membrane hydraulic conductivity and the cell volumetric elastic modulus - two physical properties of cells which influence the rate of water absorption. These measurements will be improved by use of a computer-assisted version of the pressure probe which is being constructed. The total solute concentration (osmolality) of sub-nanoliter droplets (approx. the volume of one large cell from the pea stem cortex) is being measured by cryoscopic osmometry. Current studies are aimed at determining whether cell turgor and the osmolalities of the intracellular and extracellular solutions are changed by mild water stress and, if so, how such changes relate to the reduction in growth. Future experiments will determine whether extracellular solutes serve as part of a turgor-regulating mechanism. A novel method for measuring the yielding properties of the cell wall (that is, wall extensibility and the yield threshold, or minimum turgor for cell expansion) by in vivo stress relaxation is being developed and tested. This method will be used to determine whether water stress alters cell wall properties in such a way as to inhibit growth.

69. UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

FACTORS GOVERNING LIGHT DRIVEN ELECTRON AND PROTON TRANSLOCATION IN PROTEINS ACROSS MEMBRANES $82,000
P. Leslie Dutton
Department of Biochemistry & Biophysics

Obligatory to respiratory and photosynthetic energy supply to the cell and tissue is the stage in which electron transfer and, coupled to the electron transfer, proton transfer is directed across the cytoplasmic membrane. In most membrane proteins little is known about these charge separations while in others, particularly the photosynthetic reaction center, rough details of the structural and energetic arrangements are starting to emerge. We are studying planar monolayers or proteins deposited using a Langmuir-Blodgett trough, on planer glass/electrode coated supports; these provide 10^2-10^3 times the surface density of protein encountered in the native membranes. We are measuring and manipulating electric reactions directly, with simultaneous spectrophotometric assay of the oxidation-reduction reactions. Using Langmuir-Blodgett techniques we are determining guidelines to prevent denaturation of proteins on the trough air-water interface, to obtain two-dimensional order, and to generate a greater degree of vectorial asymmetry (and therefore activity) of the protein in the films, as well as exploring different electrode materials and surfaces. We are now working mainly with the reaction centers from Rps. sphaeroides which transfer electrons (only) across the monolayers. With the native system at the current level of development, we have revealed that specific flash kinetics of the primary photosynthetic charge separative and recombination reactions can be modulated by electric fields. We are preparing to explore systems in which the native ubiquinone is replaced by quinones with systematically varying electrochemical properties, anticipating field effects descriptive of the charge separation and recombination dictated by the properties of the quinone. Fundamental insights to the function of these molecular electronic devices are anticipated. We are planning electrode design and film production for the proton pumping ubiquinol-cytochrome c oxidoreductase.

70. PURDUE UNIVERSITY, Dept. of Horticulture
West Lafayette, Indiana[1]
NATIVE PLANTS INC.; Salt Lake City, Utah[2]

REGULATION OF PROTEIN AND mRNA METABOLISM IN SALT TOLERANT AND INTOLERANT CULTURED HIGHER PLANT CELLS $79,934
R. A. Bressan[1], A.K. Handa[1], P.M. Hasegawa[1], T.H. Ulrich[2],
G.J. King[2], T. Helentjaris[2]

The objective of this project is to identify and characterize proteins and corresponding genes associated with NaCl tolerance in cultured tobacco cells. We have identified several polypeptides associated with NaCl tolerance, and the levels of some of these (58 Kd, 37 Kd, 35.5 Kd, 34 Kd, 26 Kd, 19.5 Kd and 18 Kd) increase as cells become more adapted. A 26 Kd polypeptide comprises about 10% of the total cell protein in cells adapted to 25 g/l NaCl, and is virtually absent in unadapted cells. The 26 Kd protein is synthesized in response to exogenous abscisic acid (ABA) in the presence or absence of NaCl. When exposed to NaCl, unadapted cells begin sooner to synthesize the 26 Kd protein and grow in the presence of ABA than in the absence of ABA. Both the synthesis of 26 Kd protein and enhanced tolerance to NaCl is stable for several generations when cells adapted to 25 g/L NaCl are transferred to medium without NaCl. Quantitation of the 26 Kd protein is being carried out using antibody raised against 26 Kd protein isolated and purified from NaCl adapted cells. Antibody also will be used to isolate mRNA from polysomes in an in vitro translation system. The 26 Kd protein from adapted cells is a basic protein with a PI greater than 8.0. It is a proline rich hydrophobic protein. We have determined the N-terminal amino acid sequences (first 50 amino acids) of the 26 Kd protein and a synthetic nucleotide probe will be synthesized to isolate the 26 Kd protein gene(s) from a genomic library of tobacco. Subcellular localization of the 26 Kd protein is being determined and it appears not to be associated with the mitochondria or chloroplast. The major In vitro translation products of mRNA from unadapted and NaCl adapted cells do not appear different using the rabbit reticulocyte or wheat germ system. To help identify genes whose expression is associated with adaptation, cDNA libraries from mRNA from adapted and unadapted cells were prepared and are being screened.

71. PURDUE UNIVERSITY
West Lafayette, Indiana 47907

PRIMARY GENE PRODUCTS AS PLANT DEFENSES $80,000
Donald E. Foard and Larry L. Murdock
Departments of Botany and Plant Pathology and of
Entomology

The long-term objective of this research is an understanding of the biological interaction between insect proteinases and plant proteinase-inhibitors. Our model system is the cowpea weevil (Callosobruchus maculatus) on cowpea (Vigna unguiculata). Our studies are aimed at understanding in detail: (1) the vulnerable system in the insect, i.e., the digestive proteinase; (2) the method of recruitment of proteinase activity in the feeding cycle and the effects of various inhibitors on levels of proteinase activity; (3) the chemical nature and comparative biochemistry of proteinase inhibitors; (4) the effects on growth and development of individuals and populations of C. maculatus when it eats food containing inhibitors of its digestive proteinase. These experiments can best be performed with the seed-feeding C. maculatus, which is very amenable to studies in the laboratory. In the future, we shall attempt to adapt this model system to studies of leaf and root-feeding insects representative of pests of standing biomass.

72. THE ROCKEFELLER UNIVERSITY
New York, NY 10021

NUCLEAR GENES FROM NICOTIANA ENCODING THE SMALL SUBUNIT OF $100,000
RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE
Anthony R. Cashmore
Laboratory of Cell Biology

Two nuclear genes from pea encoding the small subunit of ribulose-1,5-bisphosphate carboxylase have been isolated and characterized. In collaboration with the laboratory of Drs. Schell and Van Montagu in Gent, Belgium, we have used Agrobacterium-mediated transformation to examine regulatory sequences in these genes. A hybrid gene was constructed in which a 5' noncoding fragment from the small subunit gene SS36 was joined to the coding region of the bacterial gene encoding chloramphenicol acetyl transferase. This hybrid gene was shown to demonstrate light-inducible expression upon introduction into tobacco cells. Deletions of the 5' noncoding fragment have been prepared to further define the "inducer" sequences responsible for mediating light-induction.

A second type of hybrid genes have been constructed which contain the coding region for the small subunit transit sequence. These hybrid genes are being used in both in vitro and in vivo studies to examine the feasibility of translocating foreign polypeptides into chloroplasts.

We propose to extend the above studies by isolating small subunit genes from Nicotiana plumbaginifolia. The structure and expression of these genes will be characterized in a manner similar to our studies with the pea small subunit genes. Transformation studies with hybrid genes will also be carried out. Here, in contrast to the studies with the pea small subunit genes, we will be examining the effect of DNA regulatory sequences in their homologous cell type.

73. RUTGERS - THE STATE UNIVERSITY
New Brunswick, New Jersey 08903

CELLULASE - A KEY ENZYME IN FERMENTATION

$55,230

Douglas E. Eveleigh and James D. Macmillan
Department of Biochemistry and Microbiology, Cook College

Cellulose is a major component of biomass and a potent energy resource. In this regard, the enzyme cellulase can be employed to convert cellulose to glucose, a product that can be fermented to a variety of energy-sparing products. The focus of this project is the selective detection of cellobiohydrolase using monoclonal antibodies. Cellobiohydrolase represents a major component of the cellulolytic complex produced by *Trichodera reesei*, and currently there are no direct methods to assay for it. Thus we have prepared monoclonal antibodies against purified cellobiohydrolase of *Trichoderma reesei* RUT C-30 by fusing spleen cells from an immunized mouse with myeloma cells (P3X 63Ag8653). Forty-four groups of hybridoma cells out of 180 fusates yielded a positive antibody to cellobiohydrolase. Three different hybridomas (8B3, 2A2, IC6) were chosen for characterization. These monoclonal antibodies were able to be used to detect cellobiohydrolase in both crude and purified cellulase preparations. In comparison, polyclonal antiserum developed against cellobiohydrolase reacts both with this protein and unfortunately also with several other proteins (other cellulase components?). We are attempting to clarify these differences by *in vitro* preparation of cellobiohydrolase. Here, autoradiographs utilizing monoclonal antibodies reveal one band migrating as cellobiohydrolase whereas polyclonal antiserum reacts with an additional five proteins. These results using the monoclonal approach appear to yield satisfactory specificity and will permit development of a specific assay for cellobiohydrolase.

74. SMITHSONIAN INSTITUTION
Washington, D.C. 20560

A PRIMARY LIGHT HARVESTING SYSTEM: THE RELATIONSHIP OF PHYCOBILISOMES TO PHOTOSYSTEM I AND II

$62,162

Elisabeth Gantt
Environmental Research Center
Rockville, Maryland 20852-1773

It has long been known that energy absorbed by phycobiliproteins is transferred to photosystem II and is then distributed to I. Consequently, it has been predicted that phycobilisomes would be in close association with photosystem II. Our laboratory has succeeded in isolating phycobilisomes which have photosystem II activity, as measured by oxygen evolution, and reduction of dichlorophenol indophenol. In a special medium (0.5 M phosphate buffer, 0.5 M sucrose, 0.3 M citrate, and 10 mM magnesium chloride) the phycobilisomes remain intact, and the PS II activity is preserved. These preparations are deficient in the PS I reaction center pigment P700, as well as in the PS I polypeptide CP 1. Preparations of this system are being further characterized to determine the P680 content, to ascertain the DCMU-binding protein, cytochromes, and other polypeptides which are specific for PS II, and also for PS I. In addition, the sidedness of thylakoid membranes of red algae and cyanobacteria is being explored by immunocytochemistry (EM) and fractionation on acrylamide gels. Attachment of the phycobilisomes, and the location of the terminal emitter(s) of phycobilisomes, are integral parts of these studies. Results from these studies will aid in our understanding of the energy transfer in the photosynthetic apparatus of these groups of organisms.

75. SOUTHERN ILLINOIS UNIVERSITY
Carbondale, Illinios 62901

REGULATION OF ALCOHOL FERMENTATION BY ESCHERICHIA COLI $62,000
David P. Clark
Department of Microbiology

The purpose of this project is to elucidate the way in which the fermentative synthesis of ethanol is regulated in the facultative anaerobe Escherichia coli. We have isolated a variety of regulatory and structural mutations. In particular we have used suicide substrates of both alcohol dehydrogenase and acetaldehyde CoA dehydrogenase to isolate mutants defective in the interconversion of acetyl CoA and ethanol. Analysis of these mutants together with protein purification has suggested that alcohol dehydrogenase and acetaldehyde CoA dehydrogenase are, in fact, separate enzymatic activities of the same rotein. We are presently characterizing the ethanol synthesizing enzyme complex with respect to its tal ion requirements, pH optimum, inhibitors and molecular properties. Expression of the adhE gene ich codes for alcohol dehydrogenase and acetaldehyde dehydrogenase is under the control of the nearby adhC control region and also of the newly discovered adhR gene which is distant from the adhCE operon. The regulatory interactions which affect expression of the adh genes are being investigated by means of gene fusions. A collection of gene fusions is being accumulated, in which the gene for β-galactosidase, lacZ, is fused to promoters which are inactive aerobically but active anaerobically. In addition, suicide ubstrates of alcohol dehydrogenase are being used for the direct selection of inserts of fusion forming λ lacZ phage into the adh gene.

76. STANFORD UNIVERSITY
Stanford, California 94305

GENETIC ENGINEERING OF CORN AND OTHER HIGHER PLANTS $85,200
Ronald W. Davis
Department of Biochemistry

Our long term goal is to study and modify the expression of genes in maize. We want to understand the molecular basis for the exquisite specificity of gene expression with regard to cell type, timing during growth, pattern in tissue, amount produced, induction by hormones, and changes in response to physical and chemical stress. With this knowledge an exact program of regulation can be built in vitro for any gene to increase or decrease expression in a precise manner. We believe that modification of the expression of existing maize genes, as well as the introduction of novel genetic material, will be of great long term value in crop improvement to increase efficiency and number of usable products.

Our goal requires two research directions. First, we will analyze the structure of genes using existing and newly developed techniques for gene isolation and mapping. Second, we will analyze the function of genes in the homologous organism requiring the development of new techniques for reintroducing genes into maize.

77. STANFORD UNIVERSITY
Stanford, California 94305

DETERMINATION OF THE ROLE THAT THE ALCOHOL DEHYDROGENASE GENES (Adh1 and Adh2) PLAY IN FLOODING TOLERANCE, BY GENETIC ANALYSIS AND IN VIVO NMR SPECTROSCOPY $60,000
Oleg Jardetzky
Stanford NMR Center

The potential for using the alcohol dehydrogenase genes (Adh) and gene products as biochemical markers for the selection of crop plants with increased flood tolerance will be assessed. This will be done by defining the physiological roles that Adh1 and Adh2 play in maize plants exposed to hypoxic environments; specifically, their role in ethanol synthesis and utilization, and their relationship to flooding tolerance. We will combine a comprehensive genetic analysis with methods, principally in vivo nuclear magnetic resonance spectroscopy, to monitor the metabolic activity of roots and other organs of maize during and after flooding. In the genetic analysis, using mutants, levels of Adh1 and Adh2 gene products will be varied over wide ranges, while keeping all other genes constant. We will quantitate tolerance to flooding as the ability to recover (e.g. growth, and normal metabolic functions) after periods of flooding. ^{31}P- and ^{13}C-NMR will be used to follow critical metabolic parameters (such as intracellular pH, phosphorylation potential and energy charge, and the accumulation of toxic metabolic end products) in intact tissues; both excised tissues and tissues in whole plants will be examined. The effect of varying Adh gene product levels on metabolism during and after flooding, and on flooding tolerance, will be determined. Such an analysis will allow unambiguous assignment of the role of the Adhs gene in flooding tolerance, and so let us determine if these genes and gene products can be used as markers for selection of plants that show increased yield in areas prone to flooding.

78. STANFORD UNIVERSITY
Stanford, California 94305

CLONING AND MAPPING OF EARLY SYMBIOTIC GENES OF RHIZOBIUM MELILOTI $78,616
Sharon R. Long
Department of Biological Sciences

Biological nitrogen fixation has the potential to replace part of our consumption of energy-costly ammonia fertilizer. Symbiotic associations of Rhizobium and legumes form the most important source of agricultural biological nitrogen fixation. We are using genetics and molecular biology to study the symbiosis between Rhizobium meliloti and its plant host, alfalfa (Medicago sativa). We generated mutants of R. meliloti which cannot establish nodules on plants, and thereby identified the bacterial genes required for infection. We have used transposable elements to create 82 mutations in the nodulation DNA region, and have identified 4 complementation groups. Two of these A and B, are sharply defined and are located at the right side of an 8.7 kb EcoRI DNA fragment. Just to the left of these are two further groups of mutants: C, which is large and may contain more than one operon; and F, which contains two mutants showing a leaky (+/-) phenotype. These 4 groups of genes have been complemented by cloned nod gene DNA of other organisms, demonstrating that they are general or conserved invasion genes, rather than being used in host determination. In addition to the genes of the 8.7 kb EcoRI fragment, we have identified another nodulation gene region by complementation of mutant strain WL131. We have cloned this DNA region and have shown it is located near the other nod genes. To improve our ability to map R. meliloti genes, we have developed a transducing phage system and have demonstrated its use in correlating physical DNA distance with genetic data. We will continue to investigate the position of nodulation genes in R. meliloti during the next year.

79. STANFORD UNIVERSITY
Stanford, California 94305

CARBON DIOXIDE AND THE STOMATAL CONTROL OF WATER BALANCE AND PHOTOSYNTHESIS IN HIGHER PLANTS $80,000
Eduardo Zeiger
Department of Biological Sciences

Stomatal regulation of gas exchange in leaves has an impact on photosynthesis and plant productivity. Stomatal conductance depends on the turgor relations of guard cells, which are modulated by active ion transport in response to environmental signals. Guard cells are thus multisensory devices transducing stimuli into metabolic events which result in optimal stomatal conductances under continuously changing environmental conditions. This research is aimed at the characterization of the stomatal responses to carbon dioxide and their role in the control of stomatal conductance and its coupling with leaf photosynthesis. Recent findings in our laboratory point to the guard cell chloroplast as a receptor site for the CO_2 signal in guard cells. Immunocytochemical studies with antibodies against the CO_2-fixing enzyme RUBPcarboxylase showed that the antibodies bound to guard cell chloroplasts. The discrepancy between these data and previous biochemical studies pointing to a lack of the carboxylase in guard cell chloroplasts could indicate that the enzyme is present in an inactive form or that its activation requires hitherto undefined assay conditions. Current studies with isolated guard cell chloroplasts purified from protoplasts are providing direct evidence for photophosphorylation, a potential source of energy for stomatal opening. A modulation of photophosphorylation by CO_2 is a possible transducing mechanism for the stomatal responses to CO_2. Ongoing gas exchange studies of photosynthesis and stomatal conductance under varying CO_2 concentrations are testing these hypotheses in the intact leaf. Further progress should increase our understanding of the impact of stomatal function on plant productivity and enhance our ability to evaluate possible consequences of atmospheric CO_2 enrichment on the biosphere.

80. TEXAS A&M UNIVERSITY
College Station, Texas 77843

METABOLIC MECHANISMS OF PLANT GROWTH AT LOW WATER POTENTIALS $33,867
John S. Boyer
Department of Soil and Crop Sciences

The goal of this new project is to understand the mechanisms regulating plant productivity when water is in limited supply, i.e., when plants have low water potentials (low Ψ_w). Our investigations will be both subcellular and organismal and will involve direct measurements of tissue water status that allow comparison with work from other laboratories. We have shown that productivity is frequently regulated by photosynthesis at low Ψ_w. Chloroplasts lose activity and often cause the change in photosynthesis. We will investigate how these losses occur and what chloroplast reactions are inhibited in sunflower (*Helianthus annuus* L.). First, we will test the effects of varying the cell content of inorganic ions, particularly [illegible], and the light intensity during dehydration because previous work has implicated these factors in the chloroplast response to low Ψ_w. Second, we will investigate the activity of chloroplast partial reactions in intact leaves using several spectral techniques to determine whether effects previously observed in isolated chloroplasts reflect changes occurring *in vivo*. Cell enlargement is important for root development and the reproductive process at low Ψ_w and will be studied as well. We will focus on the primary signals that alter growth rates. Particular emphasis will be placed on tissue turgor and water potential gradients as possible candidates for the primary signal because earlier work is not in agreement about the role of turgor of Ψ_w in growth at low Ψ_w. We will use soil-grown plants as well as a seedling culture system for soybean (*Glycine max* L. Merr.) and maize (*Zea mays* L.). Growth regulator mutants will be employed to determine whether abscisic acid and gibberellic acid play a role in the primary signals or as subsequent regulators of the growth response.

81. UTAH STATE UNIVERSITY
Logan, Utah 84322

BIOENERGETICS OF THE METHANOGENIC BACTERIA — $70,000
Jack R. Lancaster, Jr.
Department of Chemistry and Biochemistry

The research in our laboratory is directed toward delineating how energy is conserved by the methanogenic bacteria. We are specifically addressing the question of how phosphorylation is coupled to the eight-electron reduction of CO_2 to CH_4 by H_2 and to the conversion of formate to CH_4. We are initially attempting to answer whether the overall mechanism is Substrate-Level Phosphorylation (SLP) or Electron Transport Phosphorylation (ETP). Our efforts presently involve determining whether transmembrane ion gradients play a primary role in methanogenesis-driven ATP synthesis. We are utilizing both whole cells and subcellular preparations of *M. voltae* and *M. thermoautotrophicum* and are measuring the effects of dissipation of ion gradients (utilizing ionophorous antibiotics) on ATP synthesis as well as examining for the presence of a membrane-bound electron transfer complex (a requirement for ETP). We are also characterizing a very active ATPase activity in *M. thermoautotrophicum*, specifically with regard to adenine nucleotide metabolism and energy coupling.

82. Washington University
St. Louis, Missouri 63130

GENETIC ENGINEERING WITH A GENE ENCODING A SOYBEAN STORAGE PROTEIN — $65,000
Roger N. Beachy
Department of Biology

The goal of this project is to identify the nucleotide sequences that regulate the transcriptional expression of a gene encoding the α'-subunit of β-conglycinin, one of the globular storage proteins of soybean (*Glycine max*). One such gene, GMg 17.1, was isolated and its DNA sequence determined. The exonuclease Bal 31 was used to resect increasing amounts of DNA sequences in front of the gene since similar experiments with other eukaryotic genes demonstrated that these sequences controlled the expression of such genes. Nine mutants containing from 30 to 850 nucleotides 5' of the gene were recovered. Each of these mutant genes, as well as the non-mutant genes, has been ligated into the plasmid pMON 200, a shuttle vector (designed by scientists at Monsanto Company, St. Louis, MO) used to transfer desired genes into the *Agrobacterium tumefaciens* Ti-plasmid. Petunia and tobacco tumor cells and plants that result from transformation experiments with *A. tumefaciens* will be used to determine the degree of, and specificity of, expression of the soybean seed protein gene in its foreign environment.

In other experiments the structural region of Gmg 171 was ligated to a transcriptional promoter from cauliflower mosaic virus, and mobilized into petunia cells via the Ti-plasmid transformation system. Transformed cells were regenerated into whole plants. Storage protein mRNA was detected in transformed cells (tumor as well as regenerated plants), and we are currently analyzing protein from tumors, and leaves and seeds of the regenerated plants to determine that the mRNA was translated. These experiments were done to verify that the gene under study is not a pseudogene and that it indeed encodes an α' subunit of β-conglycinin.

83. WASHINGTON UNIVERSITY
St. Louis, MO 63130

HYDROXYPROLINE-RICH GLYCOPROTEINS OF THE PLANT CELL WALL (HPRGPCW) $50,000
J. E. Varner
Department of Biology

Hydroxyproline-rich glycoproteins in plants apparently have structural roles and roles in cell-cell recognition. We are characterizing the chemical, physical, and biological properties of a wall hydroxyproline-rich glycoprotein that is one third protein and two thirds carbohydrate. The carbohydrate is 3% galactose and 97% arabinose. The protein is 46% hydroxyproline, 14% serine, 12% histidine, 7% lysine, 11% tyrosine and 6% valine and has an isoelectric point of about pH 11. The glycoprotein is 100% in the polyproline II conformation. It is a rigid rod 80 nm long. After secretion into the wall space the glycoprotein is slowly insolubilized apparently by the formation of isodityrosine cross-links. All preliminary evidence indicates that there are several closely related genes that may be presumed to code for several closely related precursors of hydroxyproline-rich proteins and that the bases coding for serpro$_4$ is a common sequence of these genes. The tissue distribution of the HPRGPCW promises clues about its function. All cells may have a small amount of HPRCPCW. The level increases dramatically when cells are 1) put into callus or suspension culture, and 2) when cells are wounded or infected. In seeds seed coats are by far the richest in HPRGPCW. Within the seed coat the outer one or two cell layers have the most HPRGPCW. We are 1) determing the amino acid sequence of this (these) protein(s) by a) sequencing cloned cDNA made against the purified mRNA, b) sequencing DNA from genomic clones selected by the cDNA, 2) characterizing the prolyhydroxydase that hydroxylates selected peptidylprolines, 3) trying to find which tyrosine residues are involved in cross-linking, 4) studying tissue distribution and the control of expression of the gene for this structural protein, and 5) beginning to examine the relatedness of the various hydroxyproline-rich glycoproteins.

84. WASHINGTON STATE UNIVERSITY
Pullman, Washington 99164

REGULATION OF TERPENE METABOLISM $71,344
Rodney Croteau
Institute of Biological Chemistry, 6340

Oils and resins from plants are increasingly employed as replacements for petroleum-based industrial feedstocks, and the potential for the expanded use of these renewable resources is considerable. To realize this potential, fundamental knowledge of the biochemistry of oil and resin terpenes is needed, particularly as it applies to regulatory mechanisms at the enzyme level. The objective of this research program is to provide such an understanding through the intensive investigation of two model systems (camphor metabolism in *Salvia officinalis* and menthone metabolism in *Mentha piperita*) which allow probing the control of both biosynthetic and catabolic processes involved in monoterpene accumulation. The pathways of biosynthesis responsible for the accumulation of both monoterpenes during development are now established. At maturation, menthone produced in the leaves is reduced to neomenthol which is glucosylated and transported to the rhizome. At this site the glucoside is hydrolyzed, the aglycone oxidized back to menthone and the cyclic ketone cleaved by conversion to 3,4-menthone lactone. Modified β-oxidation of the carbon skeleton of the lactone affords acetate which is employed in the biosynthesis of acyl lipids and phytosterols of the rhizome. A lactonization step is also involved in the catabolism of camphor. Monoterpene transport from mature foliage can thus be explained as providing a carbon source to the developing rhizome in which recycling to other lipids via acetate occurs. A major focus of the research is on factors which may mediate developmental changes in the rates of biosynthetic and catabolic processes. The new information gained from this investigation will have important consequences for the yield and composition of terpenoid oils and resins that can be made available for industrial exploitation.

85. WASHINGTON STATE UNIVERSITY
Pullman, Washington 99164

DNA TRANSFORMATION OF PLANT CELLS DEFECTIVE IN NITRATE REDUCTASE ENZYME ACTIVITY $45,000

Andris Kleinhofs and Paul F. Lurquin
Department of Agronomy and Soils and Program in Genetics and Cell Biology

We are cloning and characterizing the nitrate reductase genes from Escherichia coli and using these genes to transform nitrate reductase-deficient plant mutants. The objectives of this work are to develop plant cell transformation techniques by using the nitrate reduction trait as a selectable marker and to gain insight about the genetic control of nitrate assimilation in higher plants. The work to date has concentrated on the chlA locus. This gene was cloned and subcloned into two small regions each containing a different gene capable of correcting different E. coli chlA mutations. These data indicate that the chlA locus is complex and consists of at least two cistrons. One of the subclones was sequenced in order to permit construction of a hybrid gene for expression in plant cells. These constructs will be tested for transformation of nitrate reductase-deficient plant mutants. These experiments will tell us which plant genes are homologous in function to which E. coli genes. Direct hybridization homology was tested and determined to be negative. Similar work with the other E. coli nitrate reductase-deficient genes will allow us to identify the corresponding genes in higher plants. This relationship between the plant and bacterial genes is important to establish to allow more detailed investigation of these gene functions. Nitrate reductase-deficient mutants are available in dicotyledonous as well as monocotyledonous higher plants. The dicotyledonous plants can be transformed with Agrobacterium based vectors. We will use gene constructs that have been shown to work with dicotyledonous plants to learn how to transform monocotyledonous plant species. These techniques will be important in the genetic engineering of monocotyledonous species which constitute most of our major crop plants.

86. UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

STUDIES ON THE CONTROL OF PLANT CELL ENLARGEMENT BY CELLULAR PARAMETERS $67,348

Robert E. Cleland
Department of Botany

The goal of this research is to determine how plant cell enlargement is controlled at the cellular level. In many stem and coleoptile cells, the hormone auxin causes the cells to excrete protons, and the resulting lowered wall pH is then responsible for wall loosening and cell enlargement. Auxin is believed to exert this effect by activating a plasma membrane ATPase (PM-ATPase) in some fashion. We have been studying the effect of auxin on isolated PM-enriched fractions of membrane vesicles from pea roots, using fluorescence quenching to follow ATP-driven proton transport. We have demonstrated that auxin causes a significant reduction in the Km for ATP, so that the ATPase is more efficient in utilizing low levels of ATP, and have shown that this is specific for active auxins. To study this more effectively, we have been developing procedures for solubilizing the ATPases and reconstituting them into synthetic vesicles. This system has been used to study the effect of the phytotoxin fusicoccin (FC) on ATP-driven proton transport. After solubilization of membrane proteins with deoxycholate, the proteins are incubated with FC, then reconstituted into vesicles. The FC-pretreated vesicles have a significantly reduced Km for MgATP, with no change in Vmax. Our second project has been to develop a new technique for measuring the yield threshold (Y)--the turgor that must be exceeded if walls are to extend. Tissues are excised, treated for 30 min with FC, then after removal from a water source their turgor (P) is measured with a micro-pressure probe or with a psychrometer. Within 1-2 hours, P falls until it reaches Y, and then stabilizes. The growth-effective turgor (P-Y) can also be measured by this technique.

87. UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

GENETIC ENGINEERING OF YEASTS FOR FERMENTATION OF XYLOSE TO ETHANOL $70,000
Benjamin D. Hall and Clement Furlong
Department of Genetics

A major constituent of hemicellulose is xylose which occurs in all woody plant tissues. Our main objective is to construct yeast strains that are capable of growing fermentatively on xylose. Both *Saccharomyces cerevisiae* and *Schizosaccharomyces pombe* can convert the 2-ketopentose xylulose to ethanol, but are unable to ferment xylose. This is due to a natural inability to convert xylose into xylulose. The introduction of the xylose isomerase gene, which mediates this reaction, into these yeasts should enable them to grow fermentatively on xylose. We have cloned the xylose isomerase structural gene from *Escherichia coli* and determined its sequence (Schellenberg et al. JBC, in press). Direct evidence that the gene cloned codes for the xylose isomerase protein was provided by a comparison between a partial NH_2-terminal amino acid sequence and the DNA sequence which were found to be in complete agreement. The xylose isomerase gene has been fused to promoter fragments from the *ADHI* and *ADH* genes from *S. cerevisiae* and *S. pombe*, respectively. Yeast transformants containing the fused *ADH-xylose isomerase* gene have been isolated and are being studied both for the production of xylose isomerase enzyme and the ability to utilize xylose. The transformants produce detectable amounts of xylose isomerase cross reacting material as determined by Western blot analysis using antibodies raised against purified xylose isomerase protein. Studies on the pentose metabolism of these transformants are now in progress.

88. UNIVERSITY OF WASHINGTON
Seattle, Washington 98195

GENETICS IN METHYLOTROPHIC BACTERIA $70,000
Mary E. Lidstrom
Department of Microbiology and Immunology

The goal of this project is to determine the organization of genes necessary for growth on one-carbon compounds in a facultative methanol utilizer, *Pseudomonas* AM1, and an obligate methane-utilizer, *Methylosinus sporium*. We are isolating C-1 specific genes by complementing *P*. AM1 methanol mutants with clone banks constructed in broad host range vectors. The complementing clones are characterized by restriction mapping, and C-1 specific genes are defined by a combination of transposon mutagenesis and subcloning. Expression studies are being used to determine gene-polypeptide relationships. DNA-DNA hybridization will be used to compare relatedness between genes encoding similar functions in these two methylotrophs.

89. UNIVERSITY OF WISCONSIN
Madison, WI 53706

ORGANIZATION OF THE *R* CHROMOSOME REGION IN MAIZE
Jerry L. Kermicle
Department of Genetics
$40,255

Alleles of the *R* gene confer specific patterns of anthocyanin pigmentation to tissues of the corn plant and seed. We seek to identify, map and characterize the interaction between components which govern the presence, distribution, intensity, and timing of pigmentation. Mutational and recombinational analyses of alleles existing in geographically diverse races serve to characterize variation at two levels. The *R* gene is represented more than once in some alleles due to chromosome segment duplication. Each representation (genic element) functions independently, governing pigmentation of particular plant or seed parts. Individual genic elements are subdivided by recombination into regions which are responsible for the tissue-specific action of that element and other regions which can be substituted between elements of contrasting tissue-specific effects. Spontaneous mutations as well as variants isolated following chemical mutagenesis and insertion of transposable elements are utilized in the analysis. These studies provide a map of *R* pigmenting components which incorporates variation in the number and kind of genic elements. We are characterizing other phenomenon of *R* gene regulation, such as paramutation, in similar terms. We want to relate the components for such phenomena to the map of basic pigmenting determiners.

90. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

STARCH SYNTHESIS IN THE MAIZE ENDOSPERM AS AFFECTED BY
STARCH-SYNTHESIZING MUTANTS
Oliver E. Nelson
Department of Genetics
$56,303

During the past year, our major effort has been concentrated on an examination of the oligosaccharide synthase activities present in developing maize endosperms. These synthases (one starch granule-bound and the other soluble) utilize glucose-1-PO_4 as a substrate and synthesize maltodextrins of not more than ten glucose units. Our results indicate that the initial products are phosphomaltodextrins. Phosphorylase can use the oligosaccharides formed by these enzymes as primer molecules to which glucose units are added, and it is possible that these enzyme systems supply the primer molecules used by all starch-synthesizing enzymes. A report of these results is now ready for submission. The debranching enzyme deficiency in the *sugary* maize mutants has been reported in PLANT PHYSIOLOGY (1984, 74, 324-328).

91. UNIVERSITY OF WISCONSIN-MADISON
Madison, Wisconsin 53706

CARBON ISOTOPE FRACTIONATION IN PLANTS $73,500
Marion H. O'Leary
Department of Chemistry

Plants fractionate carbon isotopes during photosynthesis in ways which reflect photosynthetic pathway and environment. The object of our work is to develop methods for using this isotope fractionation to give information about how the components of the carbon fixation process (diffusion, carboxylation, etc.) vary with the species, environment, and other variables. To this end, we have developed quantitative models for carbon isotope fractionation which describe this process in terms of rates of diffusion, carboxylation, and other components. We have developed experimental approaches which focus on the initial events in carbon dioxide fixation and enable us to determine the relative rates of the various individual processes involved. We also develop other methods for using stable isotopes to study plant metabolism. We have developed an isotopic method to measure the activity of carbonic anhydrase and fumarase *in vivo* in CAM plants. We have measured the carbon isotope fractionation associated with the diffusion of CO_2 in aqueous solution. We are currently developing methods for measuring carbonic anhydrase and fumarase activity in C4 plants. We are continuing to measure the carbon isotope fractionation associated with CO_2 fixation in CAM plants in order to determine the variation in the fractionation with environment and physiology. We are also constructing a total isotopic carbon balance for CAM plants. We are also beginning studies of isotope fractionation in C4 plants.

92. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

PHYTOCHROME FROM GREEN PLANTS: ASSAY, PURIFICATION AND CHARACTERIZATION $55,000
Peter H. Quail
Botany Department

This project is directed toward assaying, purifying and characterizing phytochrome from chlorophyllous tissue of both terrestrial and aquatic plants. The approach involves (a) the use of polyethyleneimine (PEI) to remove chlorophyll from phytochrome-containing extracts, thereby permitting spectroscopic characterization; and (b) the use of immunochemical procedures coupled with proteolytic mapping for further characterization. The peak position of Pr from green *Avena* tissue is shifted some 15 nm to shorter wavelength relative to its etiolated-tissue counterpart. Western blot analysis demonstrates the presence of two species of phytochrome in this tissue: a minor polypeptide of 124 kilodaltons (kD) and a major polypeptide of 118 kD. Immunoprecipitates contain all of the 124 kD species with >95% of the 118 kD species remaining in the supernatant. The 118 kD species is structurally distinct from etiolated-oat phytochrome: peptide maps of 118 kD green-oat phytochrome are substantially different from those of etiolated-oat phytochrome and the two phytochromes exhibit differential antigenicity toward monoclonal antibodies. The significance of these data is that they indicate that green-oat tissue contains two distinct molecular species of phytochrome - a minor species resembling the 124 kD molecular from etiolated tissue and a major species previously uncharacterized.

93. UNIVERSITY OF WISCONSIN
Madison, Wisconsin 53706

MOLECULAR MECHANISM OF ENERGY TRANSDUCTION BY PLANT MEMBRANE PROTEINS

$58,401

Michael Sussman
Department of Horticulture

The focus of this project is a protein that converts chemical energy into electrical energy. This protein is known as a [H^+]-ATPase, or proton pump, and is found in the plasma membrane of fungi and higher plants. Its function is to generate a proton electrochemical gradient which is essential for the uptake of minerals and nutrients. The protein has unique molecular properties. Since it contains a single polypeptide of $M_r = 104,000$ that is phosphorylated during the reaction cycle, its chemical structure is very similar to that of cation-translocating ATPase's found in the plasma membrane of animal and bacterial cells. However, since it only translocates protons, it is functionally more similar to the membrane ATPase found in bacteria, mitochondria and chloroplasts.

In this project, protein modification and sequencing techniques are used to study how the enzyme functions. In addition to its active site involved in ATP hydrolysis, a previously uncharacterized ion binding site is being probed, using the irreversible carboxyl-modifying reagent, dicyclohexylcarbodiimide. A procedure has been developed to purify the hydrophobic ATPase and its cleaved fragments by reverse-phase high pressure liquid chromatography. By solid- and gas-phase protein sequencing techniques, the amino acid sequence surrounding this site will be determined. Current studies focus on plasma membrane H^+-ATPase purified from two species: the mycelial fungus, Neurospora crassa, and the higher plant, Avena sativa. We find that the two enzymes share similar reactivity to active-site directed reagents. Work is in progress to determine which amino acids are conserved in the sequence in the active sites of the enzyme from these two species. Results from this study will be used to define a molecular mechanism by which this protein converts chemical energy into electrical energy.

94. UNIVERSITY OF WISCONSIN-MADISON
Madison, Wisconsin 53706

ONE CARBON METABOLISM IN ANAEROBIC BACTERIA: ORGANIC ACID AND METHANE PRODUCTION

$88,000

J. G. Zeikus
Department of Bacteriology

We are engaged in understanding one and multi-carbon metabolism by acetogenic and methanogenic bacteria. Our studies with the acetogen, Butyribacterium methylotrophicum, have focused on the elucidation of the enzymes, carbon flow, and the electron and carbon carriers of the pathways of acetate and butyrate synthesis during growth on substrates such as glucose, pyruvate, methanol, formate, carbon monoxide, and hydrogen-carbon dioxide. Specifically, enzymes dealing with one carbon oxidation/reduction reactions, glycolysis, and electron transfer are being assayed in the organism after growth on various substrates. Electron carriers are being identified using spectral and chromatographic techniques. Carbon flow into end products is traced using ^{13}C nuclear magnetic resonance spectroscopy. In our studies with the methanogen, Methanosarcina barkeri, we are investigating the catabolism of acetate with a soluble in vitro system for methane production from this substrate. Using inhibitors, ^{14}C tracers, and extract fractionation, we are indentifying possible enzymes and coenzymes involved in the pathway. This work has led to a model of ATP synthesis coupled to methanogenesis from acetate. Electron flow and hydrogenase function during growth on non-gaseous substrates is also being investigated.

95. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

CHLOROPHYLL-PROTEIN COMPLEXES: PHOTOREGULATION OF TRANSCRIPTION, STABILITY AND PHOSPHORYLATION
John Bennett
Biology Department
$130,000

The objective of the research is to study the structure, function and formation of chlorophyll-protein complexes in the photosynthetic membranes of plants and cyanobacteria. These complexes catalyze the initial steps in photosynthesis: energy capture and photochemistry. Proteins to be studied include the reaction center proteins of photosystems I and II and the light-harvesting chlorophyll *a/b* protein (LHCP). Structural studies on these complexes involve several approaches: (1) gene cloning and sequencing, (2) *in situ* proteolysis and chemical labelling, (3) antibody binding, (4) binding of chlorophyll to proteins synthesized from cloned genes in *Escherichia coli* and cyanobacteria. Functional and biosynthetic studies will center on mechanisms by which light controls the organization and abundance of chlorophyll-protein complexes. Three areas of adaptive control are being explored: (1) regulation of mRNA levels, (2) regulation of protein turnover, (3) protein phosphorylation. Current studies on mRNA levels concern the role of phytochrome in regulating the expression of genes for LHCP and, for comparison, the large and small subunits of ribulose 1,5-*bis*phosphate carboxylase/oxygenase. Future work will involve mRNAs for reaction center proteins. Protein turnover is an important determinant of LHCP levels; studies deal with the identity of the photoreceptor(s) involved in stabilizing LHCP against breakdown and with characterizing the protease responsible for breakdown. Analysis of mRNA levels and protein turnover will reveal the ways in which plants adapt the composition of their photosynthetic membranes to changes in the intensity, spectral quality and daily duration of light. The ability of LHCP to donate excitation energy to the two photosystems is controlled by protein phosphorylation. Purification of the LHCP kinase will permit the study of its substrate specificity, its redox control and its location within thylakoids.

96. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

PLANT MOLECULAR GENETICS
Benjamin Burr and Frances A. Burr
Biology Department
$210,000

The primary focus of this laboratory is an investigation of the phenomena associated with the activity of transposable genetic elements in maize. These phenomena are also known in other crop plants and are of economic importance. When plants are regenerated from tissue culture, heritable variation is observed in the progeny. Mutations at the *shrunken* locus occur about ten times more frequently than in control plants. Although we have demonstrated that endogenous regulatory elements can be activated by this process, the majority of mutant alleles contain no detectable rearrangements at the DNA level. We conclude that in this system some mechanism other than transposable elements is responsible for most of the mutations. If this finding can be generalized, it means that the use of tissue culture to generate variability is much less efficient than chemical mutagenesis. Studies are continuing to determine the mechanism of mutagenesis. A high degree of variability is known to persist in some commercially imporant cultivars after many generations of inbreeding. Because the biological basis for this phenomenon is unknown, this problem leads to difficulties for seed certification. We are attempting to see if transposable elements are involved in these instabilities. *Shrunken* and *waxy* mutants have been selected in these stocks and mutant alleles are being examined at the DNA level to determine whether insertional mutations have been obtained. A mutator line has been identified by Professor D. S. Robertson at Iowa State University. Four new *shrunken* mutations generated in this stock have four different insertional elements, one of which is strain specific.

97. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

MECHANISMS OF ENERGY CONVERSION IN PHOTOSYNTHESIS $280,000
Geoffrey Hind
Biology Department

The goal of this project is to discover how energy is transformed from electron potential to chemiosmotic potential in photosynthetic systems. Processes involving cyclic electron transport are in prime concern and are studied in (1) intact chloroplasts of the C-3 plant, *Spinacia oleracea*, (2) bundle sheath cells of the C-4 plant, *Zea mays* and (3) isolated heterocysts from the filamentous cyanobacterium *Anabaena 7120*. In these systems, electron flow from reduced plastoquinone to the photochemically generated oxidant, P700$^+$, is mediated by a cytochrome *b/f* complex. The polypeptide compositions of complexes from these organisms are being compared and their activities *in situ* or following detergent extraction are being studied using flash, steady state and low temperature spectrophotometry. In cyclic flow, electrons return to the cytochrome complex *via* ferredoxin-NADP$^+$ reductase, which is non-covalently bound to its stromal surface. The structures of the complexes and binding of reductase are studied using cross-linking reagents. The protein kinase activity of reductase is being evaluated for its possible *in vivo* role in state transitions, which control apportionment of excitation energy, from light-harvesting chlorophyll, between photosystems. Passage of electrons through the complex is coupled to vectorial H$^+$ transport, possibly by a form of "Q-cycle" as postulated by Mitchell; the stoichiometry of this coupling and its dependence on ambient redox poise are being studied to elucidate the coupling mechanism. These investigations will provide knowledge of the factors limiting photosynthetic reduction of CO_2 and N_2. In showing how the cytochrome complex serves as an efficient energy transformer, they are also of presumed relevance to future design of biomimetic energy conversation devices.

98. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

THE CHARACTERIZATION OF MODIFIED T-DNA GENES AND HOW THEY ARE EXPRESSED IN TRANSFORMED PLANT TISSUE $150,000
Daniela Sciaky
Biology Department

The T-DNA of *Agrobacterium tumefaciens* provides an excellent model system for the study of how genes are expressed in plants. We are studying two spontaneous mutations in the *tms* locus of the T-DNA, both which result in the formation of tumors that make shoots. One spontaneous mutation has occurred in the T-DNA after transformation of *Nicotiana otophora* by pTiB6806 and has resulted in the deletion of a region of the *tms* locus of the T-DNA. The second mutation is due to the insertion of IS66, a 2.5 kb insertion sequence, in the T-DNA of pTiA66. The site of insertion of IS66 has been localized to within the structural region of the gene for *tms* transcript 2. Sequencing of IS66 has shown that it contains several open reading frames, including one frame that is 1600 nucleotides in length. Studies are now underway to determine whether IS66 is transcribed in plants and whether it can act as a transposable element in plants.

99. BROOKHAVEN NATIONAL LABORATORY
Upton, New York 11973

THE PHYSIOLOGY AND BIOCHEMISTRY OF CYANOBACTERIA $200,000
Harold W. Siegelman
Biology Department

Cyanobacteria are cosmopolitan organisms of soils, marine, and freshwaters. They are frequently responsible for water blooms and can cause serious water management problems in rivers, lakes, and reservoirs. The success of cyanobacteria in nature is probably associated with an efficient photosynthetic mechanism, frequent possession of gas vacuoles permitting vertical migration in the water column, and ready adaptability to varying environmental factors. The molecular structure and composition of the photosynthetic energy collection systems including phycobilisomes, chlorophyll proteins, and carotenoids are being characterized in several cyanobacterial species. Phycobilisomes from cells grown at several light intensities and spectral qualities are purified by hydrophobic-interaction chromatography, salt precipitation, and gel chromatography. Their apparent mass and structure are being characterized by electron microscopy, gel permeation, and absorbance spectroscopy. HPLC and rapid scanning spectrophotometry will be used to determine the phycobiliprotein stoichiometry of the phycobilisomes. Three-dimensional space-filling models of phycobilisomes are being constructed by computer. Antibodies to highly purified phycobiliproteins are being raised to initiate a molecular biology examination of the control mechanisms regulating phycobilisome composition. Cyanobacteria grown at several light intensities and qualities show profound morphological and fine structure changes which are being examined by electron microscopy. HPLC methods are used to purify the peptide toxins of Microcystis aeruginosa. They are also being used to develop a quantitative analytical assay for the toxins. The pathological and hematological effects of the toxins are being examined with mice.

100. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

LIGHT REGULATION OF NUCLEAR AND CHLOROPLAST GENE EXPRESSION IN Euglena gracilis $55,000
James C. Bartholomew
Laboratory of Chemical Biodynamics

Even though the chloroplasts of photosynthetic organisms contain their own genome, many of the functions carried out in the organelle are encoded in the nucleus. Some of the proteins which function in chloroplast are encoded partially in the chloroplast and partially in the nucleus. The expression of both these genomes is regulated by light. Light stimulates mRNA synthesis as well as DNA synthesis in Euglena gracilis. Presumably, this light response is mediated by photopigments in the cells which receive the light and convert it into a signal which controls nucleic acid activity in both the genome compartments. We have a series of bleached mutants of Euglena which lack various photopigments as well as have different levels of chloroplast DNA. We are using these mutants to study the involvement of the photopigments and chloroplast DNA in the stimulation of nuclear DNA and RNA synthesis. First, we are characterizing the cell cycle response of these various mutants by flow cytometry. Wild type Euglena conditioned in the resting medium in the dark can be stimulated to reenter the cell cycle by light. We are comparing the kinetics of reentry into the cell cycle of the bleached mutants with that of the wild type to discern the role of the chloroplast supplied functions in regulating the DNA replication response in the nucleus. We are also comparing the light stimulated expression of nuclear encoded chloroplast functions in the wild type vs bleached mutants to determine if the chloroplast plays a role in the regulation of the nuclear genes. We have begun to map the nuclear genes for the light harvesting chlorophyll a/b proteins in Euglena to determine if polymorphisms exist for this/these polypeptide(s). All of these studies are designed to help us understand the factors involved in the coordinate regulation of the genes in the two physically distinct compartments.

101. LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA, Berkeley, CA 94720

PLANT BIOCHEMISTRY: REGULATION OF PHOTOSYNTHETIC METABOLISM AND SECONDARY BIOSYNTHESIS — $352,000
James A. Bassham, Henry Rapoport
Chemical Biodynamics Division, Lawrence Berkeley Laboratory

The objectives of this project are to determine photosynthetic and biosynthetic paths in green plants and the mechanisms of regulation in these paths. Both metabolic regulation (feedback inhibition, energy charge, etc.) and regulation of gene expression are studied in plant tissue, including whole plants and organs, cells and organelles isolated from leaves, and plant tissue culture. Subtask I (Regulation of Metabolism and Gene Expression) focuses on key enzymes and processes of metabolism in photosynthetic cells, and is directed to obtaining a better understanding of control of primary carbon and nitrogen metabolism in these cells. Gene expressions resulting in syntheses of pyruvate phosphate dikinase (PPDK) and of isoforms of phosphoenolpyruvate carboxylase (PEPC) are examined as a function of C_4 and C_3 metabolism, tissue type (leaf and seed), and conditions of cells in tissue culture (whether differentiating or non-differentiating). In the case of PPDK, *in vitro* translation of mRNA from plant tissues and determination of molecular weight of the resulting polypeptide is used to determine whether chloroplast or cytoplasmic type PPDK is being expressed. Subtask II (Secondary Plant Metabolism: Plant Pigments) includes similar goals focussed on secondary products and also investigation of structures and mechanism of action of non-chlorophyllous plant pigments.

102. LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

MOLECULAR GENETICS OF THE PHOTOSYNTHETIC GENES OF *RHODOPSEUDOMONAS CAPSULATA* — $133,000
John E. Hearst
Chemical Biodynamics Division

The goal of this project is a detailed molecular understanding of the primary chemical events in the storage of light energy by the photosynthetic purple non-sulfur bacterium, *Rhodopseudomonas capsulata*. In our initial efforts to achieve this goal we have sequenced the genes for the reaction center subunit polypeptides H, M, and L. Comparison of these sequences with those of the psbA and psbD loci of the chloroplast genomes of *Chlamydomonas reinhardii* and of these same loci in higher plants such as spinach and pea has established that the D1 and D2 chloroplast proteins which are coded by these loci contain sequences of 31 amino acids about 60% in from the amino termini of these proteins which are similar to the sequences at the same positions which we determined in the L and M subunits of the bacterial reaction centers. We have postulated that these sequences, which have been conserved during the three billion years of evolution since the divergence of the purple non-sulfur bacteria and higher plants, are functionally related to quinone binding in the reaction centers of these bacteria as well as the reaction centers of photosystem II in photosynthetic eukaryotes. We have synthesized nucleic acid oligonucleotides which code for these two highly conserved sequences and we intend to probe for equivalent genes in a number of other photosynthetic species, including the thermophilic cyanobacterium *Synechococcus sp*. and perhaps the primitive organism *Chloroflexus aurantiacus*. The objective here is establishing the phylogenetic relationships between the many photosynthetic organisms. We are engaged in a study of quinone binding and electron transport in the isolated *R. capsulata* reaction center complexes of wild type and mutant strains. We are continuing to generate photosynthesis mutants which we typically generate by Tn5.7 transposon mutagenesis. The physical characterization of these mutants is being worked on in collaboration with the laboratory of Professor Kenneth Sauer.

103. LAWRENCE BERKELEY LABORATORY
Berkeley, California 94720

CHARGE SEPARATION IN THE PHOTOSYNTHETIC LIGHT REACTIONS $290,000
Kenneth Sauer, Melvin Klein
Chemical Biodynamics Division

The photosynthetic light reactions begin with the absorption of photons by chlorophyll and other pigment molecules followed by transfer of excitation to reaction centers where primary charge separation takes place. We are measuring the time course of these processes in the picosecond to microsecond time domain using fluorescence decay kinetics and time-resolved electron paramagnetic resonance (EPR) spectroscopy. The fluorescence decay from intact photosynthetic membranes consists of several exponential components that fall into two classes: those yields that are sensitive to the open or closed state of the reaction centers and those that are not. The insensitive components, which are typically faster (50-500 ps) reflect excitation loss during the process of transfer from the pigments that absorbed the light toward the reaction centers. Under favorable circumstances we have also been able to detect the rise or induction of this fluorescence, which is a direct indication of these transfer times. We are seeking to understand the mechanism of this excitation transfer process. By combining the observations of reaction center-sensitive fluorescence with measurements of the kinetics of appearance and decay of characteristic EPR signals, we can monitor the initial stages of the charge separation process. In this manner we have identified several of the molecular components involved in the reaction center complexes. Through analysis of the amino acid sequence of the reaction center polypeptides from the photosynthetic bacterium *Rps. capsulata* and comparison with that from a chloroplast thylakoid protein, we have identified a distinctive oligopeptide segment that we believe is the binding site for quinone electron acceptors. We hope to determine the important aspects of intermolecular interactions and geometric relations that enable these photosynthetic components to function with very high energy conversion efficiency.

104. LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
Berkeley, California 94720

PHOTOCHEMICAL CONVERSION OF SOLAR ENERGY $117,000
Lester Packer, Rolf J. Mehlhorn, Alexandre T. Quintanilha
Membrane Bioenergetics Group, Applied Sciences Division

The goal of this research is to identify the molecular mechanism of the photochemical activity of bacteriorhodopsin, an extremely stable and simple energy-transducing membrane protein which directly couples absorption of visible light to the production of proton and electrical gradients across membranes of halobacteria. Bacteriorhodopsin is studied in its natural membrane, in isolated purple membrane sheets and after reconstitution into liposomes. In the next phase of research, the role of light-induced surface potentials will be further defined and compared by using an ESR spin probe method and laser Doppler velocimetry (electrophoretic light scattering). In native and chemically modified purple membranes, carboxyl groups will be cross-linked to lysine residues under conditions favoring either intra- or intermolecular bonds to study the effect of conformational constraints on function and the relationship of molecular segments to one another. Chemical modification and cross-linking studies of the hydrophilic tail of bacteriorhodopsin will be undertaken to determine its involvement in function. If there is a precise stoichiometry for proton release and uptake by bacteriorhodopsin, correlating with the photocycle, then it will be possible to formulate molecular mechanisms. Results to date indicate variable stoichiometry for purple membranes in suspension. We have recently shown, by quasi-elastic light scattering and electron microscopy, that purple membranes are rarely in suspension as free flattened sheets, but more often exist as stacks of membranes. A thorough investigation of factors which effect the uniformity of purple membranes in suspension will allow more accurate measurement of the stoichiometry.

105. LAWRENCE BERKELEY LABORATORY
University of California

RESONANCE STUDIES IN PHOTOSYNTHESIS
Alan Bearden
Division of Biology and Medicine

$64,000

This research is aimed at understanding the biophysical processes important to both primary reactions in green-plant photosynthesis and electron-transfer in subsequent "dark" bioenergetic electron-transport. Techniques include electron paramagnetic resonance and optical spectroscopy. Continuing experiments using laser-initiated photochemical conversion and oriented chloroplast membrane fragments and reaction-center mutants of Chlamydomonas are underway in an effort to gain further information about the order of photochemical reactants (donors and acceptors) and their inter-relation. Tunneling as a method of electron-transfer has long been implied in bioenergetic reactions in both photosynthesis and other pathways. Following a successful demonstration of a Hopfield charge-transfer band in Chromatium (Proceedings of the National Academy of Sciences 81, 135-139 (1984)) we are continuing both theoretical and experimental studies of the role of multicomponent vibrational systems in biophysical processes. These more physical studies may have a range of applicability in such seemingly disparate topics as enzyme specificity, fundamental limits on energy-transduction processes, and the role of coherence in light absorption by important macromolecules.

106. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ANALYSES OF PHOTOSYNTHETIC MEMBRANES
Charles J. Arntzen
MSU-DOE Plant Research Laboratory

$215,000

The goal of our research is to identify cellular factors which limit biomass productivity by limiting the quantum efficiency of photosynthesis (especially in plants growing in non-optimal environments). Our approach is to use biophysical and biochemical analyses for characterization of isolated photosynthetic membranes from green plants, algae, and photosynthetic bacteria. We have devised protocols which allow us to subfractionate these membranes so that individual pigment-proteins (chlorophyll and carotenoids non-covalently associated with unique polypeptides) and enzymatic complexes can be purified and characterized. We are particularly interested in the genetic controls which regulate synthesis, turnover, and post-translational modification of these membrane components. Our current research emphasis is to characterize cellular controls of the stoichiometry of pigment-proteins and reaction center components of chloroplast membranes, and to define mechanisms which regulate the assembly of supramolecular protein complexes in these membranes. The long range goal of these efforts is to identify genetic or cultural means by which photosynthetic efficiency can be increased, especially in plants suffering from environmental stress. Our shorter term emphasis is in three specific areas. We are investigating: a) the polypeptides of the photosystem II complex of higher plant chloroplasts which participate in the water oxidizing reactions of photosynthesis; b) the assembly and post-translational modifications of the chlorophyll b-containing light-harvesting pigment proteins; and c) the properties of quinone binding proteins of photosynthetic membranes with special emphasis on the molecular characterization of quinone or quinone analog "target sites".

107. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

DIFFERENTIAL GENE EXPRESSION IN *RHIZOBIUM* $165,000

Barry Chelm
MSU-DOE Plant Research Laboratory

The interaction of bacteria of the genus *Rhizobium* with a legume host to establish a symbiotic, nitrogen-fixing relationship requires a series of developmental steps in both the bacterium and the host plant. The objective of this project is to identify the underlying molecular mechanisms by which the expression of the bacterial genome is regulated during this process. We have focused on the *R. japonicum*/soybean system. Specific genes whose expression is regulated during nodule development or by other physiological changes and genes involved in the regulation of these expression changes have been isolated. These genes have been isolated either by hybridization screening procedures utilizing analogous genes from other organisms as hybridization probes or by complementation of genetically defective bacterial strains by cloned *R. japonicum* DNA. The genes isolated thus far include those encoding the nitrogenase subunits, glutamine synthetase I, the large subunit of ribulose bisphosphate carboxylase, delta-aminolevulinate synthetase, adenylate cyclase, and a nif regulatory gene termed nifA. The expression patterns and structures of these genes are being further characterized. Promoter regions are being localized by S1 protection analysis and the nucleotide sequences of these regions are being determined. In addition, *R. japonicum* strains carrying mutations in these genes are being constructed by site-directed mutagenesis procedures in order to more precisely define their roles in nodule differentiation, nitrogen fixation and physiological adaptation as a whole. These further understandings of these processes should enlighten the viewpoint from which the symbiotic relationship might be further optimized and manipulated.

108. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

RESISTANCE OF CROP PLANTS TO ENVIRONMENTAL STRESS $160,000

Andrew D. Hanson
MSU-DOE Plant Research Laboratory

This project concerns three metabolic pathways that are activated by stresses: betaine synthesis, promoted by water-and salt-stress: lactate synthesis, induced by O_2-deficit; and gramine synthesis, elicited by high temperature stress. These stress-activated pathways may be metabolic adaptations for coping with stress; if we knew this to be true, and if the pathways were understood genetically and biochemically, natural or induced genetic variation for such pathways could be useful in breeding stress-resistant crops. (1) Betaine. To evaluate the adaptive worth of betaine accumulation, barley isopopulations high and low in betaine are being developed, in order to test their performance under salt-and water-stress. We are also screening an M_2 population of barley for betaine nulls. The biosynthesis of betaine is being studied by supplying the precursor [^{14}C]choline to spinach leaf protoplasts and subcellular fractions therefrom. We have found that chloroplasts oxidize [^{14}C]choline to betaine, and that this oxidation is promoted by light. We are now attempting to isolate the choline-oxiding system from chloroplasts. (2) Lactate. We have shown that anaerobic barley roots can accumulate lactate, and that these roots have anaerobically-inducible lactate dehydrogenase (LDH) activity which can be resolved on native gels into a set of isozymes. We will produce polyclonal antibodies against LDH, in order to investigate synthesis of LDH peptides during anaerobiosis, and to help in the future isolation of plant *Ldh* genes. (3) Gramine. The indole alkaloid gramine is a defensive compound found in barley leaves; it is derived from tryptophan via a pathway that includes two N-methylation steps. Heat stress increases N-methyltransferase (NMT) activity specific for these steps. We are attempting to purify the NMT activity, firstly to find whether there are separate NMT's for the two methylation reactions and secondly in order to produce antibodies.

109. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ACTION AND SYNTHESIS OF PLANT HORMONES $210,000
Hans Kende
MSU-DOE Plant Research Laboratory

The principal objective of this task is to gain knowledge on the mode of action of the plant hormones ethylene and cytokinin. These hormones regulate processes related to stress and senescence in plants. Ethylene promotes aging and the appearance of stress symptoms, cytokinins retard them.

a) Regulation of stress-ethylene synthesis. Plants under stress produce ethylene. Ethylene synthesis is very rapidly induced through the enhancement of the activity of 1-aminocyclopropane-1-carboxylate (ACC) synthase. This enzyme is *de novo* synthesized during induction of ethylene synthesis. Research will mainly concentrate on the mechanism by which ACC synthase is regulated. Antibodies against ACC synthase will be produced for the isolation and further characterization of the enzyme. Using these antibodies, we shall also study the level of control of this enzyme and the mode of its turnover. We are also studying the conversion of ACC to ethylene. We were able to show that this reaction proceeds in isolated vacuoles. We are now trying to define the nature of the ethylene-forming system and we are trying to reconstitute it from homogenates. Ethylene action is being studied in rice where ethylene induces rapid growth.

b) Localization of the site of action of cytokinins. We are synthesizing a cytokinin photoaffinity probe, 8-azido-N^6-benzyladenine, in radioactive form to localize the site of action of this hormone. This will be attempted using two plant systems: moss protonemata and cultured tobacco cells. Cytokinins induce bud formation in mosses and are accumulated by target cells of this organism. In tobacco cells, cytokinins regulate cell division. We shall attempt to isolate the tagged receptor from both types of cells in order to characterize it and localize it in the cell. Ultimately, we hope to find out how cytokinins delay senescence and couteract symptoms of plant stress.

110. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

CELL WALL PROTEIN $125,000
Derek T.A. Lamport
MSU-DOE Plant Research Laboratory

Our major goal is elucidation of the role played by the hydroxyproline-rich cell wall glycoprotein extensin. Recently we demonstrated *in muro* pools of two monomeric extensin precursors (designated P_1 and P_2), and a new crosslinked amino acid, isodityrosine (IDT) present in extensin, but absent from the precursors. This led to the "warp-weft" model of the primary cell wall which postulates a highly crosslinked extensin network ("weft") penetrated by a cellulose microfibrillar "warp".
We propose to characterize the "warp-weft" model by sequencing the monomeric extensin precursor to determine probable crosslink domains and their frequency, hence defining network porosity.
Other approaches involve attempts to establish a precursor crosslink-generating system *in vitro* so that, by subtractive peptide mapping, we can compare this with partially crosslinked extensin extracted from growing cell walls. We shall also attempt direct electron microscopic and *in muro* electron microscopic observation of extensin precursor and crosslinked extensin, moving towards the ultimate question: Do cellulose microfibrils indeed penetrate the pores of a highly crosslinked protein network?

111. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

REGULATION OF FLOWERING $90,000
Anton Lang
MSU-DOE Plant Research Laboratory

This program deals with regulation of flower formation by hormone-like (i.e. translocatable) substances, the current main focus being on inhibitors of flower formation ("antiflorigen"). The existence of antiflorigen has been conclusively demonstrated, in previous research under this program, by grafting experiments. Antiflorigen, like the promotive hormone-like factor(s) of flower formation ("florigen, floral stimulus"), is not specific in either the taxonomic or the physiological sense, being interchangeable between different species and genera, and between plants in which flowering is dependent on different environmental (photoperiod) conditions. This physiological evidence strongly indicates that both antiflorigen and florigen are ubiquitous in flowering plants, at least monocarpic herbaceous ones. The next logical step would be isolation and chemical identification of these compounds. We are currently working on this problem with emphasis on antiflorigen, since - among various reasons - solution of this problem may be helpful in the search for florigen, which so far has been unsuccessful. In addition, work has been initiated with several inhibitors of gibberellin biosynthesis (growth retardants), which have recently become available and are considerably more effective than those previously used, in order to determine to what extent gibberellins are essential in the regulation of flower formation.

112. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

INTERACTION OF NUCLEAR AND ORGANELLE GENOMES $165,000
Lee McIntosh
MSU-DOE Plant Research Laboratory

In the development and maintenance of a photosynthetic apparatus in higher plants and other photosynthetic organisms there is an ordered series of events which lead to the ability to form complex carbon compounds from gaseous carbon dioxide and light energy: photosynthesis. The scope of the research involved in this task is to understand the underlying mechanisms of gene regulation, especially those genes whose products are involved in photosynthetic reactions, and to develop methods which make it possible to approach the future improvement of heritable characteristics in higher plants. This research is designed to delineate: 1) The molecular mechanisms by which the genomes of the nucleus and chloroplast control the development and maintenance of photosynthetic competence in higher plants. 2) The molecular/genetic basis for the relation of structure to function in photosynthetic polypeptides involved in electron transport, initially Photosystem II (PS II). 3) The structural basis for catalysis of the primary "dark-reaction" enzyme Ribulose 1,5-bisphosphate carboxylase/oxygenase. 4) Development of a photosynthetically assayable system of site-specific gene modification on higher plant and cyanobacterial genes involved in photosynthesis.

113. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ACQUISITION OF ENVIRONMENTAL INFORMATION THROUGH LIGHT PERCEPTION $125,000
Kenneth L. Poff
MSU-DOE Plant Research Laboratory

The ultimate goal of this work is an understanding at the molecular level of sensory transduction in plants from stimulus to response. Our emphasis is on non-visual light perception and temperature perception. We are studying the "blue light" photoreceptor system which controls numerous light responses such as phototropism in plants and the phytochrome photoreceptor system which regulates plant photomorphogenesis by using specific inhibitors and genetic mutants as probes blocking specific initial steps in the transudction sequence. Light direction is measured in plants through a photochemical measurement of light intensity on the two sides of the plant. Understanding this aspect requires knowing the internal light intensities. Since direct measurement is intrusive, and models difficult due to the absorption and scattering complexities of the tissue, we are developing techniques for using an internal physiological pigment such as phytochrome as a physiological quantum counter which can in turn be asayed using microspectrophotometry. Isolation and analysis of photoreceptor pigment mutants which will permit dissection of the transduction sequence are in progress for Arabidopsis, corn, and Dictyostelium.

Thermotaxis by Dictyostelium is being used as a model system for the study of temperature perception because of four unique characteristics: (1) the extreme sensitivity to temperature, (2) the narrow temperature range over which temperature is measured (3) the dependence of the thermotaxis range on the previous growth temperature, and (4) the fact that thermotaxis can be observed in individual cells.

114. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

PHYSIOLOGICAL AND MOLECULAR GENETICS OF HIGHER PLANTS $175,000
C.R. Somerville
MSU-DOE Plant Research Laboratory

The overall objective of this task is to develop genetic systems for the analysis and modification of specific physiological processes in higher plants. We are using this conceptual framwork to investigate several distinct aspects of plant biology in which single gene variation may be a strong determinant of plant productivity.

A) Based on the premise that photorespiration is deleterious to net photosynthesis we are attempting to create useful or informative variation in the enzyme RuBP carboxylase/oxygenase by in vitro modification of the genes which encode the enzyme. We are also attempting to resolve several uncertainties in our model of photorespiration by the isolation of specific classes of mutants in Arabidopsis thaliana which are theoretically possible but have eluded discovery.

B) Although genetic variation in disease resistance is available in many species, it is not known what the genes for resistance encode. The concept that plant cell-surface receptors are an important component of some classes of host defense mechanisms is well established. In the context of this theory, we are exploring the possibility that hybridoma techniques can be used to define and characterize the biochemical differences between disease-resistant and suceptible cultivars of barley.

C) As part of a study of several mutants of Arabidopsis with altered chilling sensitivity, we have isolated a novel series of mutants of this species which appear to specifically lack certain fatty acid desaturases. We are attempting to determine the precise biochemical defect, and are examining the effect of the resulting changes in lipid composition on membrane associated functions and on the growth and vigor of the mutants in various environmental conditions.

115. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

DEVELOPMENTAL BIOLOGY OF NITROGEN-FIXING ALGAE $160,000
C.P. Wolk
MSU-DOE Plant Research Laboratory

Certain cyanobacteria (blue-green algae) trap solar energy via photosynthesis and utilize the resulting chemical reducing power to fix atmospheric nitrogen gas (N_2). They thereby produce ammonia, which then is utilized as the nitrogen source for cellular growth. The initial steps of N_2 assimilation take place in specialized cells called heterocysts. The objective of this project is principally to understand the supply of energy and electrons to, and the oxygen protection of, nitrogen fixation within heterocysts. Our current approach makes use of our recently developed methodology for introducing cloned genes into nitrogen-fixing cyanobacteria by conjugation from *Escherichia coli*, and is primarily genetic. That is, we are developing methods, using site-specific mutagenesis and transposons, for isolating mutants of *Anabaena* and *Nostoc* defective in cellular differentiation, nitrogen fixation and photosynthesis. Additional, simpler, more rapid means for introducing genes into *Anabaena* are being sought, as are means for visualizing transcriptional differences between cells cooperating in N_2 fixation. With partial support from N.S.F., we are also constructing a physical and genetic map of the *Anabaena* genome using the technique of cosmid walking. Thus, we have made substantial progress toward developing tools for genetic analysis of photoautotrophic, nitrogen-fixing cyanobacteria. The significance of this work is that it opens the way to increased understanding of cellular differentiation and to construction of modified strains which would be particularly suitable for commercial application of biological solar energy conversion.

116. MICHIGAN STATE UNIVERSITY
East Lansing, Michigan 48824

ENVIRONMENTAL CONTROL OF PLANT DEVELOPMENT AND ITS RELATION TO PLANT HORMONES $160,000
Jan A. D. Zeevaart
MSU-DOE Plant Research Laboratory

Environmental factors such as daylength, temperature and moisture have pronounced effects on growth and development of plants. Plant hormones often function as chemical messenger between the perception of an environmental factor and the morphological expression. The objectives of this task are to characterize the hormones involved, how their synthesis and catabolism are regulated by the environment, and how these hormones act. Topics under investigation are: (1) Stem growth and flowering in rosette plants, the so-called "physiological dwarfs", as regulated by gibberellins (GAs). We know that in spinach the conversion of GA_{19} to GA_{20} is under photoperiodic control. The immediate objective is to prepare a cell-free system that catalyzes this step, and then to determine how the activity of the enzyme is regulated by the daylength. (2) In single-gene dwarf mutants of tomato and *Arabidopsis* we will determine which steps in the gibberellin biosynthetic pathway are blocked. This will be done by feeding various precursors and GAs. Furthermore, endogenous GAs of the wild type will be identified and compared with the GAs in the mutants, if detectable at all. (3) Regulation of abscisic acid (ABA) synthesis, catabolism, and distribution. We are measuring early changes in apoplastic ABA in *Xanthium strumarium* leaves to see if this parameter is more closely related to stomatal aperture than bulk leaf ABA during the onset of water stress. Since our earlier work suggests that stress-induced ABA is not directly produced from mevalonic acid, we are investigating the possibility that xanthoxin, a breakdown product of xanthophylls, is the precursor of ABA.

117. OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831

ENERGY AND NUTRIENT UTILIZATION EFFICIENCY IN INTENSIVE FOREST BIOMASS PRODUCTION $200,000

S. B. McLaughlin, D. W. Johnson, N. T. Edwards,
R. J. Luxmoore, Environmental Sciences Division

The primary objective of this work is to provide physiological criteria for quantifying yield potential of biomass candidate species, to determine the role of soil-plant nutrient dynamics on productive potential of these species, and to provide important insights into the physiological basis of species' tolerance and adaptability to environmental stress. Four tree species, yellow poplar (*Liriodendron tulipifera*), loblolly pine (*Pinus taeda*), sweet gum (*Liquidambar styriciflua*), and black locust (*Robinea pseudoacacia*) are being studied in a 20 ha managed plantation. Treatments being examined include mycorrhizal preconditioning, variable rate and timing of nitrogen supply, and mulching. Plant physiological parameters being measured include whole tree allocation of energy between metabolic pools, plant water status, leaf photosynthetic rate, photosynthate allocation by foliage, and root and soil respiration rate. The kinetics of nitrogen mobilization, and movement through soil-plant nutrient cycles, are being examined to quantify nutrient conservation mechanisms under varying rates of nutrient supply. These data will provide important insights into the interactions involved in seasonal allocation of carbon, water, and nutrients for representative biomass candidate species and aid in the selecting of criteria for enhancing biomass production potential. Biochemical analysis of tissues from 147 trees sampled during the 1983 growing season is in progress. Quantification of seasonal changes in sugars, lipids, starch, cell wall, and lignin in tissues will be used to compare energy allocation patterns between species and treatments. In studies of nitrogen kinetics, principal effects of intensive nitrogen fertilization have been found on soil nitrification potential but little effect on nitrogen mineralization rates has been noted to date.

118. SOLAR ENERGY RESEARCH INSTITUTE
Golden, CO 80401

BASIC PHOTOBIOLOGY RESEARCH $105,000

Michael Seibert, Paul F. Weaver, and Stephen C.T. Lien
Photoconversion Research Branch

Three areas associated with photobiological H_2 metabolism will be studied. Task 1 will determine the degree of integration among H_2 metabolism, N_2 fixation, photosynthesis, and the multiple energy-conversion mechanisms present in photosynthetic bacteria, particularly *Rhodopseudomonas* and *Rhodospirillum* species. A broad spectrum of mutants is being examined with defective redox components operative in autotrophic or heterotrophic, anaerobic or aerobic, and light or dark growth modes. These defects are being characterized by pleiotropic losses of other growth modes, spectral and enzymatic properties, and protein separation and quantitation techniques. The data will be used to amplify H_2 evolution in organisms which utilize two distinct evolving hydrogenases as well as nitrogenase. Task 2 has lead to the first purification of hydrogenase from a eucaryotic source (*Chlamydomonas reinhardtii*). Kinetic studies of the isolated enzyme will examine the role of positively charged groups on the interaction between hydrogenase and its electron mediators. New efforts will elucidate the mechanism of anaerobic activation of the enzyme. The role of iron in the activation and catalysis reactions of algal hydrogenase will be examined. Task 3 will investigate physicochemical and structural properties of Photosystem II (PS II) in algae, chloroplasts, and detergent-fractionated PS II preparations that maintain O_2-evolving capacity. Work will emphasize extraction of several extrinsic proteins associated with O_2-evolution and examination of the properties of the extracted membranes. Antibodies to the proteins will be produced for structural studies. New research will be initiated to examine a recently recognized intrinsic protein that may be part of the O_2-evolving complex.

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APPENDIX 4

DOE/ER-0210

Summaries of FY 1984 Research in High Energy Physics

December 1984

U.S. Department of Energy
Office of Energy Research
Office of High Energy & Nuclear Physics
Division of High Energy Physics
Washington, D.C. 20545

FOREWORD

The U.S. Department of Energy, through the Office of Energy Research, Division of High Energy and Nuclear Physics, provides approximately 90 percent of the total federal support for high energy physics research effort in the United States. The High Energy Physics Program primarily utilizes four major U.S. high energy accelerator facilities and over 90 universities under contract to do experimental and theoretical investigations on the properties, structure, and transformation of matter and energy in their most basic forms.

This compilation of research summaries is intended to present a convenient report of the scope and nature of high energy physics research presently funded by the U.S. Department of Energy. The areas covered include:
1) conception, design, construction, and operation of particle accelerators;
2) experimental research using the accelerators and ancillary equipment;
3) theoretical research; and 4) research and development programs to advance accelerator technology particle detector systems, and data analysis capabilities. Major concepts and experimental facts in high energy physics have recently been discovered which have the promise of unifying the fundamental forces and of understanding the basic nature of matter and energy.

The summaries contained in this document have been reproduced in essentially the form submitted by contractors during FY 1984 and have been edited only for format and clerical errors.

SUMMARY DESCRIPTION OF THE DEPARTMENT OF ENERGY HIGH ENERGY PHYSICS PROGRAM

Introduction

The High Energy Physics program supports basic research which seeks to discover the fundamental constituents of matter and to understand the laws of nature that govern the fundamental behavior of matter and energy. Discoveries and new knowledge resulting from past activities of this type have laid the foundation for much of the highly technological world in which we live today. During this century, scientific investigation has advanced to studies of ever more fundamental constituents of matter, with the frontier moving from research on molecules to atoms, to nuclei, to the constituents of nuclei (protons and neutrons), and recently to even more elemental subnuclear constituents called quarks and gluons.

The Department of Energy provides over 90 percent of the Federal support for this most basic scientific endeavor and serves as the Executive Agent for the national program. The Department has responsibility for planning for the national program, with the goals of achieving a comprehensive and productive national program and maintaining a competitive world leadership position for the United States.

DOE High Energy Accelerator Facilities

To probe deep into the depths of matter, into the domain of quarks and gluons, it is most effective to use intense beams of very energetic particles (electrons, positrons, protons, antiprotons) which are only available from high energy particle accelerators. Through studying the results of the violent collisions of these accelerated particles with other particles either in a dense fixed target or in another beam, information is acquired about the constituents of those particles and about the forces which act within and between them. The high energy particle accelerator and colliding beam facilities operated by the Department include: the 30 GeV (billion electron volt) proton synchrotron, Alternating Gradient Synchrotron (AGS), at Brookhaven National Laboratory (BNL); the 1000 GeV Tevatron superconducting magnet proton synchrotron at Fermi National Accelerator Laboratory (Fermilab), which will have both fixed target research capability and 1000 GeV on 1000 GeV proton-antiproton colliding beam capability; and the 32 GeV linear electron accelerator at the Stanford Linear Accelerator Center (SLAC). SLAC also has three electron-positron colliding beam facilities for which the linear accelerator serves as an injector: the Stanford Positron Electron Asymmetric Ring (SPEAR) (4 GeV on 4 GeV), the Positron-Electron Project (PEP) (15 GeV on 15 GeV), and the SLAC Linear Collider (SLC), which will have 50 GeV on 50 GeV electron-positron colliding beam capability. Each of these DOE accelerator centers provides a unique set of experimental research capabilities, complementary to the others. As an ensemble they provide the capabilities for a comprehensive forefront national research program in high energy physics.

A major part of the funding of the high energy physics program is required to meet the direct needs of the accelerator laboratories to develop, maintain, and operate the major accelerator, colliding beam and detector facilities. The facilities at these laboratories are the source of experimental data for accelerator-based high energy physics research, more than 75 percent of which is carried out by university-based scientists. In this sense, much of the funding provided to the accelerator laboratories can be considered as indirect support of the university research programs.

At Fermilab, the world's first high energy accelerator using superconducting magnets is in routine operation delivering beam to a number of fixed target experiments at 800 GeV. Extensions are being made under the Tevatron I and Tevatron II construction projects. The Tevatron I project, which provides the capability for operating the superconducting synchrotron as a 1000 GeV on 1000 GeV proton-antiproton colliding beam storage ring, is scheduled for completion in FY 1986. A key element of Tevatron I, an intense source of antiprotons, is scheduled to begin first operating tests late in FY 1985. The project remains on schedule and within cost, with first research utilization at low luminosity expected to begin late in FY 1986. The Tevatron II project, which is being completed in stages, is scheduled for full completion by the end of FY 1985 and will provide a number of new and upgraded secondary beam enclosures and experimental halls for fixed target research programs.

At SLAC, the principal emphasis in recent years has been the systematic study of electron-positron collisions at center of mass energies between 4 GeV and 30 GeV. An extension of this capability to 100 GeV center-of-mass energy will be provided by the Stanford Linear Collider (SLC). This project also has, as a primary goal, the development and demonstration of the fundamental technical feasibility of using linear accelerators with precisely controlled, high intensity, micron-sized pulsed beams to provide a reliable source of high luminosity electron-positron collisions. The successful demonstration of the SLC capabilities is a critical step toward future electron-positron colliders at energies far beyond those which would be affordable with circular colliders. SLC construction is planned on a three year schedule which will give the U.S. an operational 50 GeV on 50 GeV electron-positron collider by FY 1987, providing earliest access to the scientifically exciting physics made possible by the anticipated copious production of the Z° boson in high energy electron-positron collisions. Pre-operating systems tests of SLC are planned to begin late in FY 1986.

Future Plans--The Superconducting Super Collider

The highest priority for new high energy physics facilities is a large accelerator collider. The new facility, designated as the Superconducting Super Collider (SSC), is envisioned as a proton-proton collider with an energy of 20 TeV per beam and high luminosity, up to $10^{33}\text{cm}^{-2}\text{sec}^{-1}$. Recent rapid progress in particle physics understanding and in accelerator technology, including the great success of the CERN laboratory in its successful construction and operation of a proton-antiproton colliding beam capability and the subsequent discovery of the W and Z particles, has emphasized the importance of physics experiments in the mass range up to several trillion electron volts (TeV) where new phenomena, including new forms of matter with unique properties, are firmly expected. The SSC would have immense physics potential for truly major advances in understanding the fundamental nature of matter. It would operate in an energy domain where there are no existing or planned facilities anywhere in the world, and it would assure a world competitive U.S. high energy physics program from the mid-1990's into the next century. Such a project lies within the reach of present technology, and has been made possible by the recent outstanding successes resulting from the substantial U.S. investment in superconducting magnet technology.

Preliminary R&D related to the SSC was initiated in FY 1984. This work included R&D on technical options (particularly with regard to superconducting magnets), cost reduction studies, and reference design studies to establish technical feasibility and develop credible preliminary cost and schedule estimates. Research and development activities planned for FY 1985 include further R&D on three different superconducting magnet design concepts to determine which would yield the best performance for the SSC at the lowest cost; studies to refine the definition of the scope of the SSC, to develop a cost-optimized design, and to develop better cost and schedule estimates; and studies to establish site criteria.

The confluence of several factors served to stimulate interest in the SSC project. First, operation of the Fermilab Energy Saver has emphatically demonstrated that a superconducting accelerator will work. Recent monumental physics discoveries at CERN have shown that experiments can be performed with colliding proton beams at an energy approaching that suggested for a super accelerator. Most important, the veil has begun to lift on the physics of the future and a host of questions lie waiting for such a super accelerator.

Other DOE-Supported High Energy Physics Research

In addition to research carried out using high energy accelerators in the U.S., the Department's high energy physics program supports some experiments which use the capabilities of unique foreign accelerators and also some experiments which do not require beams from particle accelerators. The research carried out at facilities overseas takes advantage of unique research opportunities offered by foreign accelerator facilities which have capabilities not available in the U.S. The research using particles from nonaccelerator sources includes studies of very rare processes such as the predicted decay of the proton and searches for neutrino mass and isolated magnetic poles. The proton decay experiments, for example, employ large detector systems located in deep underground locations to provide an environment free from background radiation.

Summary

The High Energy Physics program may be considered to consist of three subparts: Physics Research, Facility Operations, and Accelerator R&D. Although the three functions within the program are discussed as separate subprograms, they are not independent. Each is coupled to the other two and cannot exist separately. The high energy physics program supports numerous research contracts in which there is substantial cost sharing by the universities. The universities' contributions are provided by a number of mechanisms, for example, salaries to investigators, provision of facilities, computer time and/or equipment, etc. The high energy physics program encourages such cost sharing policies to achieve maximum utilization of available Federal funds. In addition, there is cost sharing in a number of experiments by foreign participants, including substantial contributions to major detectors, such as the CDF detector at Fermilab.

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PART I

MAJOR ACCELERATOR LABORATORIES

ARGONNE NATIONAL LABORATORY
Argonne, Illinois

Award No.: W-31-109-ENG-38

Title of Project: Nucleon Decay Experiment

Person in Charge: D. Ayres

Scientific and Professional Staff: D. Ayres, K. Coover, J. Dawson, T. Fields, M. Hill, J. Hoftiezer, A. Mann, E. May, L. Price, K. Sivaprasad, and J. Thron

Scope of Work

This project is being carried out in collaboration with the University of Minnesota, Tufts University, Oxford University, and the Rutherford-Appleton Laboratory in order to build an 1200-ton detector to search for nucleon decay. The detector will be located in an underground laboratory at the Soudan iron mine in northern Minnesota. It will use iron as the source of decaying nucleons and as the calorimeter material in a large fine-grained tracking calorimeter instrumented with drift tubes. The device will provide bubble-chamber-like event reconstruction, an enormous aid in rejecting background and in extending the search beyond the simple decay modes to which current experiments are sensitive.

In addition to testing the predictions for nucleon decay of grand unified theories, this detector will be an important tool in the study of cosmic-ray phenomena.

Goals and/or Major Results to Date

Since 1980, participants in this project have been collaborating with a University of Minnesota group on a 30-ton prototype experiment to search for nucleon decay, Soudan 1. Results on this and on magnetic monopole flux limits have been published and data on cosmic-ray muon-bundle phenomena are in the final stages of analysis.

Prototype work on the long drifting structures to be used in the 1200-ton Soudan 2 detector was completed in 1983-1984, following extensive testing in the Argonne Intense Pulsed Neutron Source-High Energy Physics charged-particle test beam. The start up of module production facilities in the U.S. and U.K. will be major activities in 1984. Turn on of the first few hundred tons is expected in 1986 with completion in 1987.

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Title of Project: Polarized Beam Experiments

Person in Charge: A. Yokosawa

ARGONNE NATIONAL LABORATORY
Argonne, Illinois

Scientific and Professional Staff: R. Ketzler, D. Hill, R. Miller, H. Spinka, R. Stanek, D. Underwood, R. Wagner, and A. Yokosawa

Scope of Work

Participants in this project study polarization phenomena in high energy scattering, continuing their pioneering work in this area which began at the Argonne Zero Gradient Synchrotron (ZGS) accelerator. Argonne is leading an international collaboration to provide and use a polarized beam as part of the new fixed-target Tevatron II facilities at Fermilab. This project also relies on Facilities R&D work at Argonne to develop new polarized targets. The beam is generated through the parity-violating decays of Λ ($\bar{\Lambda}$) hyperons and will be unique as the only high energy polarized proton (antiproton) beam in the world. The first round experiment will measure total cross section differences for pure helicity states and asymmetries in the inclusive production of a variety of particles.

Goals and/or Major Results to Date

The analysis of data taken with polarized proton beam operation of the Argonne ZGS will be completed in 1984. The results include studies of spin effects in two-body reactions and establish an amplitude analysis for nucleon-nucleon scattering at high energy. They also provide important insight into the existence of di-baryon resonance states.

The design for the Fermilab polarized beam is completed and fabrication of equipment for the beam and experiment has started. Argonne responsibilities include: modification of existing beam line components and fabrication of specialized beam doagnostic equipment; provision of wire chambers for the spectrometer and also a part of the polarized-target system. The beam is expected to be completed in 1986, and the first experiment should begin in 1987.

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Title of Project: e^+e^- Collider Physics

Person in Charge: M. Derrick

Scientific and Professional Staff: M. Derrick, P. Kooijman, J. Loos, B. Musgrave, L. Price, J. Schlereth, K. Sugano, J. Weiss, and D. Wood

Scope of Work

This project uses the High Resolution Spectrometer (HRS) at the Positron Electron Project (PEP) to study the annihilation of e^+e^- into leptons and into quarks and gluons and their materialization into hadrons. The detector facility uses the superconducting magnet of the ANL 12-foot bubble chamber and was built over the period 1978-1981 in a collaborative effort between physicists from Argonne, Indiana University, LBL, the University of Michigan, Purdue University, and SLAC. The detector elements include: high precision drift chambers to track charged particles inside the magnetic volume; a segmented system of barrel and end cap lead-scintillator calorimeters, incorporating an array of proportional wire tubes, to provide triggering, time-of-flight measurement, $e^{\pm}$ tagging, and photon energy and position measurements; a Cerenkov counter system in which the Cerenkov radiation is detected through photo-ionization for identification of low energy electrons and for K/π separation. The HRS has a momentum resolution σ_p/p of 1 percent at 10 GeV/c and affords a unique opportunity for precision spectroscopic studies of hadronic or leptonic states produced up to the highest PEP energies.

Goals and/or Major Results to Date

Since startup of the facility in 1981, about 200 pb^{-1} of luminosity has been logged. Results from these data include: precise spectroscopic studies of D^* and D mesons with measurement of the charm quark fragmentation function over the full Z range (using the cascade decay $D^{*+} \to D^0\pi^+$) and first observation of a direct D signal, in both charged and neutral modes, in the PEP energy range; a measurement of the electroweak asymmetry for charm quark production; observation of the F meson by its $\phi\pi$ decay mode and measurement of the fragmentation function; detailed studies of jet fragmentation; measurements of single particle distributions for π, K and p; limits for production of scalar electrons; and measurements of Bhabha scattering and of the reactions $e^+e^- \to \mu^+\mu^-$, $\gamma\gamma$.

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Title of Project: Fixed-Target Jet Studies

Person in Charge: T. Fields

Scientific and Professional Staff: R. Ditzler, T. Fields, and G. Thomas

Scope of Work

This experiment studies the production of jets with large transverse momentum in fixed-target hadron-hadron interactions at Fermilab. The apparatus, built by an Argonne-Fermilab-Lehigh-Pennsylvania-Rice-Wisconsin collaboration, includes a precision hadron calorimeter with full azimuthal coverage, as well as magnetic analysis over a large solid angle. A principal goal is to make a quantitative study of the dynamics of quark-quark and quark-gluon scattering. In addition, nuclear target data will be used to search for new effects which might be due to quark-gluon plasma formation.

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Goals and/or Major Results to Date

The final run on this experiment (E609) was concluded in the 1983-1984 Fermilab Tevatron operating period. Analysis of data from initial running in 1982 has established, for the first time, clear evidence for the observability of jet production at Fermilab energies and has also yielded absolute values for di-jet production cross sections. With an order of magnitude increase of beam delivered on target in the recent run, values of P_T beyond 10 GeV/c can be reached. Analysis of these data will continue over the next year or two.

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Title of Project: Polarized Target Development

Person in Charge: D. Hill

Scientific and Professional Staff: D. Hill

Scope of Work

This project is presently aimed at providing targets which can fully exploit the polarized beam facility at Fermilab. The effort proceeds on two fronts; improvements in target materials and development of the hardware for a large dilution-refrigerator-cooled, frozen spin target configuration.

Goals and/or Major Results to Date

Target material research to date has concentrated on the study of high-hydrogen content substances which form glassy solids. Materials with a figure-of-merit 2.5 times greater than that of traditional ones have been found; ongoing refinements in FY 1984 promise to increase this by a further 25 percent. Deuterated analogues of these materials are being explored. Target hardware development, in collaboration with the Saclay Laboratory, is aimed at producing an operational target for the Fermilab polarized beam by late 1985.

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Title of Project: Collider Detector Facility (CDF)

Person in Charge: R. Diebold

Scientific and Professional Staff: R. Diebold, E. May, L. Nodulman, J. Proudfoot, P. Schoessow, D. Underwood, R. Wagner, and A. B. Wicklund

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Scope of Work

Participants in this project are collaborating with Fermilab and other groups in the construction of a solenoidal detector with sophisticated calorimetry in order to study $\bar{p}p$ collisions made available by the Tevatron I construction project. The major Argonne CDF activity is the production, testing, and calibration of the central electromagnetic calorimeter modules. These modules will be completed early in FY 1985. A first engineering run of the detector is expected as early as mid-1985, followed by physics studies of $\bar{p}p$ collisions at what will be the highest energy source of manmade interactions for many years. Some examples of the physics objectives include: study of the intermediate vector bosons; production of heavy quarks and leptons; and searches for other heavy new particles such as those predicted by technicolor models. The device will also be sensitive to intriguing new effects suggested by cosmic ray experiments.

Goals and/or Major Results to Date

Fabrication of the detector began in FY 1982 with Argonne having the specific prime responsibility for the central electromagnetic calorimeters and for coordinating the contributions of other groups which directly affect the shower counters. The hybrid design of the shower counter with both scintillator and wire chamber readout was made at Argonne; the suitability of this design was subsequently demonstrated with beam tests of a prototype. Fabrication of the 50 shower counter modules was half completed by mid-1984. Detailed tests of the completed modules, using both a cosmic ray test stand and a test beam at Fermilab, are proceeding in parallel with the fabrication. The CDF project is expected to be a long-term program with data collection beginning in 1986 and continuing with various detector upgrades into the early 1990's.

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Title of Project: Theory

Person in Charge: D. Sivers

Scientific and Professional Staff: A. Axelrod, E. Berger, G. Bodwin, E. Braaten, E. Kovacs, J. Ralston, D. Sivers, A. White, and C. Zachos

Scope of Work

This program covers basic theoretical physics research in the field of high energy physics. Much of this work is in collaboration with university physicists; the group plays an active role in the Chicago-area theory community and is highly interactive with experimentalists at Argonne and elsewhere.

Besides purusing theoretical physics research, participants in this program serve on committees at the local and national level; they also organize workshops and symposia on topical areas of high energy physics.

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An active visitor program is maintained which includes national and international theorists and a substantial summer program is organized in cooperation with the Division of Educational Programs at Argonne.

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Title of Project: Accelerator R&D

Person in Charge: J. Simpson

Scientific and Professional Staff: Y. Cho, S. Kramer, R. Martin, J. Simpson, and D. Suddeth

Scope of Work

The major accelerator R&D activity is the collaboration with Fermilab on stochastic cooling for the Tevatron I project. They have continued the development and operation of the unique beam pickup test and measurement facility created for this activity at the Argonne 22 MeV electron linac. Advanced microwave techniques are being developed which may permit improved TeV I performance and may be necessary for an eventual $\overline{p}$ source for the Superconducting Super Collider (SSC). Participants in this activity, together with others at Argonne, are also actively pursuing several aspects of the R&D program including work on intersection region parameters, injector parameters, superferric magnet design, and instrumentation techniques.

Goals and/or Major Results to Date

The unique beam pickup test facility which utilizes the special high current, short pulse characteristics of the Argonne 22 MeV electron linac has provided essential measurements and evaluations of prototype stochastic cooling pickups for the Fermilab antiproton source (TeV I). ANL plans further exploitation of this valuable resource with studies of wakefield acceleration cavities and of developing a fibre optics delay line for use in extremely samll dispersion comb filters, an alternative to use of superconducting coaxial lines in stochastic cooling systems.

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Title of Project: Fundamental Nonaccelerator Physics

Person in Charge: R. Hagstrom

Scientific and Professional Staff: J. Clausing, R. Hagstrom, A. M. Rushton, and J. VanPolen

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Scope of Work

Recent work under this activity has centered upon three topics: the experimental investigation of quark confinement by a search for the existence of free fractional charges in stable matter; development of a high-confidence, large-area detector to search for magnetic charges; and the design of a large supercomputer with unique architecture aimed at addressing the computational needs of problems such as lattice gauge calculations. This project also uses the resources of the high energy physics facilities R&D program.

Goals and/or Major Results to Date

The fractional charge search apparatus has been operated successfully in calibration mode and full operation is expected soon using ethylene glycol. Future plans extend the search to samples of materials enriched in abundances of fractional elements on the basis of unique chemical and physical properties of fractionally charged ions.

In collaboration with a group at LBL, a large array of sensitive ionization detectors is being used to search for slow, heavy particles, both magnetic monopoles and those which only carry electric charge; such particles might be the "missing dark matter" of astrophysics. Prototype work using microprocessors developed and demonstrated an extensible computer architecture suitable for lattice gauge calculations. A major new initiative deriving from this is the acquisition of several STAR Technology ST-100 processors by the Laboratory which, together, have the memory and rate capability of two CRAY-1 machines. While their potential is great, these parallel processors are not easy to use, and considerable effort will be needed to make them useful for lattice gauge theories. It is expected that this work can be readily extended to larger arrays of processors.

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Title of Project: Experimental Support Group

Persons in Charge: K. Coover and J. Dawson

Scientific and Professional Staff: J. Dawson, K. Coover, and N. Hill

Scope of Work

Participants in this project provide design support in the areas of electronic systems and mechanical engineering to the various experiments in the Argonne high energy physics program and assure optimal use of the technical staff in this program.

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Goals and/or Major Results to Date

All of the experiments now in progress have obtained major support from this group. During FY 1984 and FY 1985 major commitments include electronics and mechanical design for the Soudan 2 1200-ton nucleon decay experiment, electronics design for the polarized beam experiment (E704) at Fermilab, and support for an advanced computer project on extendable array processor architecture.

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Title of Project: Computer Support Group

Person in Charge: E. May

Scientific and Professional Staff: J. Clausing, E. May, A. M. Rushton, and J. Schlereth

Scope of Work

This activity advises and assists with the programming needs of the various experimental projects in the high energy physics program. This includes management of the several computers in the program and support for data acquisition and analysis.

Goals and/or Major Results to Date

Specific accomplishments of this group during 1983-1984 include installation of a VAX 11/730 for a multi-user, CAMAC-based data-acquisition system; installation and operation of a loosely coupled system of five VAX 11/750's with Ethernet-DECNET communication to the VAX 11/780 of the HRS experiment at SLAC, and support for an advanced computer project to develop array processor architecture suitable for fundamental physics application such as lattice gauge calculations.

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Title of Project: Particle Detector Development

Persons in Charge: D. Ayres and L. Price

Scientific and Professional Staff: D. Ayres and L. Price

Scope of Work

A broad program of detector development activities is supported to ensure that instrumentation for the various experimental projects takes advantage of the latest technical advances. A charged-particle test beam at the 500 MeV Argonne proton synchrotron of the Intense Pulsed Neutron Source (IPNS) facility is maintained and is used for testing new detector concepts.

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Goals and/or Major Results to Date

The development of improved calorimetric techniques using ionization sampling and tracking in gas for the Soudan 2 detector was pursued both at Argonne and at Oxford during 1982-1983 with the emphasis at Argonne being on planar long-drift chamber designs. A prototype 2 ton calorimeter was constructed and successfully tested in the IPNS test beam.

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BROOKHAVEN NATIONAL LABORATORY
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Award No.: DE-AC02-76CH00016

Title of Project: Omega Group

Persons in Charge: H. A. Gordon and S. H. Aronson

Scientific and Professional Staff: N. Baker, S. U. Chung, P. L. Connolly, B. Gibbard, T. Ludlam, M. Murtagh, V. A. Polychronakos, S. D. Protopopescu, D. C. Rahm, P. Rehak, M. Sakitt, I. Stumer, M. Tanaka, M. Tannenbaum, S. Terada, D. P. Weygand, D. H. White, C. Woody, T. Erickson, W. Gubler, and M. Montag

Scope of Work

This group conducts research in experimental elementary particle physics and in detector development. The experiments are performed at the BNL AGS as well as at CERN and Fermilab. At the AGS current experiments are in neutrino interactions, rare K^+ decays, and the hadronic production of the E(1420). At CERN an experiment is in preparation for beams of hadrons and light ions. At Fermilab there has been analysis of exposures of the 15' bubble chamber filled with heavy neon and a new major commitment to the D-Zero detector at the Tevatron-I collider. The group has the capacity for the design and construction of major pieces of apparatus. Support is given for the physics justification of the projects of the Laboratory. The detector research is now focused on silicon detectors and calorimeters.

Goals and/or Major Results to Date

The name of the group recalls the discovery of the Ω^- which occurred in the 1960's. More recently the group has discovered the first charmed baryon, measured dilepton events in ν interactions, measured $\nu_e e^-$ elastic scattering, searched for ν oscillations. Single particle spectra were measured at large transverse momenta from π and p beams yielding information on the structure functions. An anomalous e^+e^- signal was studied in π^-p interactions. Single direct γ's and jets, were discovered at the Intersecting Storage Rings while Drell-Yan e^+e^- and inclusive π^0 cross sections were measured. Searches for narrow states in $\bar{p}p$ and charm production at AGS energies were made.

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Title of Project: Alternating Gradient Synchrotron (AGS) Operations and R&D

Persons in Charge: H. W. Foelsche, D. I. Lowenstein, and P. J. Reardon

Scientific and Professional Staff: L. Ahrens, J. Alessi, D. Barge, D. Barton, J. Brodowski, G. Cornish, E. Dale, R. Frankel, W. Frey, J. Gabusi, S. Giordano, J. W. Glenn, J. Grisoli, H. Halama, A. Hershcovitch, K. Hillman, H. Hseuh, P. Ingrassia, E. Jablonski,

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S. Kennell, J. Keohane, V. Kovarik, A. Kponou, R. Lambiase,
R. Larson, Y. Lee, R. Lockey, A. Maschke, A. McGeary, A. McNerney,
P. Montemurro, M. Month, A. Otis, K. Prelec, L. Ratner, R. Reece,
L. Repeta, E. Rodger, J. Ryan, R. Sanders, J. Skelly, T. Sluyters,
L. Smith, A. Soukas, R. Thern, J. Tuozzolo, W. Van Zwienen,
R. Warkentien, R. Witkover, S. Yamin, and P. Zuhoski

Scope of Work

The Alternating Gradient Synchrotron (AGS) is a 30 GeV proton accelerator which provides high energy particles for physics experiments. The AGS Division operates the 200 MeV injector, the synchrotron itself, and the external beam systems up to and including the primary beam target stations.

The Division is responsible for accelerator studies directed toward proper operation of the AGS for utilization with the growing experimental program and for potential long-range use of the AGS as an injector synchrotron. The design, development, fabrication, and installation of new equipment and improvements to the AGS to match the experimental program are included in this activity as well as the routine maintenance and minor repairs required.

The 200 MeV linac, in addition to serving as an injector for the AGS, continues to serve satellite programs using the Brookhaven Linac Isotope Producer (BLIP) and the Chemistry Linac Irradiation Facility (CLIF). Neutron rich isotopes are being studied with use of both primary proton and secondary neutron bombardment schemes. Radioisotopes are produced on a regular weekly basis for use in clinical studies in various research hospitals.

Goals and/or Major Results to Date

The AGS ran for a scheduled High Energy Physics program of 32 weeks in FY 1984, providing both a fast extracted beam for neutrino experiments and slowly extracted beams for counter-electronic experiments. The peak AGS intensity during the period was 1.6×10^{13} protons per pulse and the average intensity was significantly higher than in any previous period.

Accelerator improvements included the further development of the new H^- ion source, the set up of the charge exchange injection system into the AGS and adiabatic improvements in the rf system, resulting in a 50 percent increase of proton intensity. Another major effort was the design, construction, and commissioning of the polarized proton capability in the AGS. The physics program will run with about 10^{10} polarized protons per pulse.

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Title of Project: Experimental Facilities Operations

Persons in Charge: D. I. Lowenstein and G. Bunce

Scientific and Professional Staff: T. Blair, H. N. Brown, G. Bunce, A. Carroll, I. Chiang, L. Chimienti, G. Danby, B. DeVito, J. Gould, F. Heimburger, R. Imossi, J. Jackson, D. Lazarus, W. Leonhardt, Y. Makdisi, J. Mills, C. Pearson, A. Pendzick, D. Pope, J. Sandberg, W. Sims, G. Smith, A. Soukas, J. Walker, and C. Zein

Scope of Work

The Experimental Planning and Support (EP&S) Division serves the AGS experimental program. All experimental beams and target stations are designed, installed, operated, and maintained by the Division.

The EP&S carries out the design, setup, and rearrangements of beams, radiation shielding and experimental devices; maintenance and operation of beam separators and cryogenic targets; measurements of magnet characteristics; the installation and maintenance of electrical power and cooling water systems, all as required to support the research activities of guest and resident scientist users.

A liaison physicist and an engineer from the Division are assigned to each experiment. They assist with the design of equipment and with its safe installation at the AGS. Liaison physicists are frequently experimental collaborators and occasionally principal investigators on AGS experiments. This has often been extremely helpful to outside user groups.

Operational crews are maintained on a 24 hour, seven-days-a-week basis to operate, service, and provide safety surveillance of the experimental areas and equipment. The EP&S Division provides liaison between BNL and the university users. Weekly "Time Meetings" of BNL personnel and users are held to discuss the schedule of beam time, intensity, and priority allotted to each experiment. Emphasis is given to being able to deliver beam to several experiments simultaneously, thus making efficient use of the AGS protons.

Goals and/or Major Results to Date

In FY 1984, 18 experiments will have taken beam in 32 weeks of running with beams from five target stations. Up to eight experiments can run simultaneously. A varied physics program includes high energy physics, nuclear physics, a QED measurement, and materials science. Examples are neutrino-electron elastic scattering which is a sensitive measure of the electroweak mixing angle, CP violation in $K \rightarrow 2\pi$ decays, gluonium searches, hypernuclear spectroscopy, inclusive and exclusive measurements with the polarized proton beam, and a sensitive measurement of the QED vacuum polarization term in muonic helium.

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Several major experimental areas will have been completed in FY 1984. A large neutrino oscillation experimental area has been completed one kilometer from the AGS and the experiment has observed neutrinos from the AGS. A new narrow band horn will be completed along with a new target hall to accommodate higher intensity. The line leading to the neutrino target will be upgraded with new optics and dipoles. Two rare K decay experiments will be installed, requiring one new secondary beam line and experimental area. There are also a large number of beam changes and experiment installations required in response to the needs of the running program.

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Title of Project: High Energy Particle Physics Research

Person in Charge: T. F. Kycia

Scientific and Professional Staff: E. J. Bleser, I. H. Chiang, R. A. Johnson, K. K. Li, L. S. Littenberg, A. Stevens, R. C. Strand, and C. I. Pertridou

Scope of Work

The group had developed differential Cerenkov counters for secondary beam particle identification for the AGS and Fermilab. These were used to measure various total cross sections to a very high precision. Another activity has been a study of rare K^+ meson and K^0_L meson decay. Searches have been carried out for hadronically produced η^c and the six-quark exotic particle, the H.

Currently, the group is preparing to study rare K^+ meson decay into a π^+ meson and noninteracting neutral particles. K^+ mesons will be stopped in the center of a large one Tesla solenoidal magnet which will contain all the detectors. These will consist of a fiber scintillator target, a cylindrical drift chamber, a scintillator range stack for π^+ meson identification, and gamma detectors for common decay rejection.

Goals and/or Major Results to Date

Refinements in the method of total cross section measurement led to the first observations of numerous resonances and structures. These were observed in $\pi^\pm$ meson, K^+ meson, and antiproton interactions on nucleons at the AGS.

Measurements at Fermilab showed, for the first time, that π^+ meson, π^- meson, and K^- meson total cross sections on nucleons were rising with energy.

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In a 4000 event sample of $K^{\pm} \rightarrow \pi^{\pm}\pi^{0}\gamma$, direct gamma emission was observed and possible CP nonconservation was ruled out. In another experiment direct gamma emission was also observed in 1070 of $K^{0}_{L} \rightarrow \pi^{+}\pi^{-}\gamma$ events. Decays $K^{0}_{L} \rightarrow e^{+}e^{-}\gamma$, $\mu^{+}\mu^{-}\gamma$, and $\pi^{\pm}\pi^{0}e^{\mp}\nu$ were observed for the first time.

In the next rare K^{+} meson decay experiment, the $K^{+} \rightarrow \pi^{+}\nu\bar{\nu}$ will be studied to test the standard model. A search will be conducted for other possible decays into a π^{+} meson and a variety of neutral, light, and weakly interacting particles such as axions, familons, and the supersymmetric photino, goldstino, and scalar Higgs.

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Title of Project: High Energy Particle Physics Research

Person in Charge: L. B. Leipuner

Scientific and Professional Staff: R. C. Larsen and W. M. Morse

Scope of Work

This group has, in the recent past, been studying CP violation. They have searched for manifestations of such violation in K decay processes other than the decay $K_{L}^{0} \rightarrow 2$ pions; examined the polarization of the μ meson in $K^{0} \rightarrow \pi^{-}\mu^{+}\nu$ and $K^{+} \rightarrow \pi^{0}\mu^{+}\nu$; and examined the charge ($\pi^{+}\pi^{-}$) to neutral ($\pi^{0}\pi^{0}$) ratio for both K_{L}^{0} and K_{S}^{0}. They are now implementing an experiment to search for the rare (or nonexistent) decays $K \rightarrow \mu + e$ and $K \rightarrow e + e$. They have also developed Brookhaven FASTBUS, a fast data acquisition system, and have used it in two major experiments. All of these efforts have been done in a long standing collaboration with a group from Yale University.

Goals and/or Major Results to Date

Polarization results indicate no new CP violation processes. BNL has pushed this limit down considerably. The not yet completely analyzed charged to neutral ratio work is of comparable accuracy to a similar experiment done elsewhere but with different systematic errors. The preliminary result is that there is no difference in this ratio for K_{L}^{0} and K_{S}^{0}. The rare decay experiment should find these processes if the branching ratio is $> 10^{-11}$.

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Title of Project: MPS II Facility (High Energy Particle Spectrometer Group)

Persons in Charge: S. J. Lindenbaum and K. J. Foley

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Scientific and Professional Staff: S. E. Eiseman, A. Etkin, C. L. Jacobs, R. S. Longacre, W. A. Love, T. W. Morris, E. D. Platner, and A. C. Saulys.

Scope of Work

The MPS facility is a large solid angle multiparticle magnetic spectrometer. It contains a hydrogen target, unique state-of-the-art drift chamber detectors, and particle identification and triggering elements. It is analogous to a high rate ($\sim 2 \times 10^6$ incident particles/sec), high resolution electronic bubble chamber with incident particles identified. The forward-going produced particles are also identified, and sophisticated, very selective trigger logic is employed. A data handling and on-line computer is provided as part of the system. The High Energy Particle Spectrometer Group designed, built, and operates the MPS II as a user facility which now serves physics groups and graduate students from approximately ten institutions. The program is, at present, devoted entirely to hadronic physics, mainly in the soft QCD area where searches for glueballs and meson resonant states are performed. Since its first successful running in the spring of 1982, the MPS II facility has been in great demand and continuously has a large backlog of approved experiments.

Goals and/or Major Results to Date

MPS II has successfully completed:

1. A glueball search in the Zweig suppressed channel $\pi^- p \rightarrow \phi\phi n$ which led to the probable discovery of one to three $J^{PC} = 2^{++}$ glueballs.

2. A high statistics investigation of the production of charged D and E mesons in $\pi^- p \rightarrow \left(\begin{smallmatrix} D \\ E \end{smallmatrix}\right) + N$ and in $\bar{p}p$ interactions to see whether glueball states occur in this reaction.

3. The radiative decay of hyperons has been studied.

4. An investigation of neutral mesons in the reaction $\pi^- p \rightarrow K_S^0 K_S^0 \pi^0 n$ is being performed to search for glueball states. Glueball states are also being looked for in $\pi^- p \rightarrow K_S^0 K_S^0 n$. All of these programs and others are expected to be pursued in second generation experiments.

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Title of Project: High Energy Theory Group

Person in Charge: M. Creutz

Scientific and Professional Staff: L.-L. Chau, M. Creutz, A. Gocksch, W.-Y. Keung, C.-S. Lim, W. Marciano, I. Muzinich, M. Ogivlie, F. Paige, C. Rebbi, G. Senjanovic, and R. M. Sternheimer

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Scope of Work

The members of this group pursue basic theoretical research in elementary particle physics. This work ranges from abstract analysis of quantum field theories to phenomenological studies of recent experimental results. Substantial benefits arise from interdisiplinary areas in which the Brookhaven condensed matter and/or nuclear theory groups have common interests. Advanced computational techniques are followed in the context of applications to numerical simulations of quantum fields.

A summer visitor program provides an informal environment for outside theorists to interact with each other and the Brookhaven staff.

Goals and/or Major Results to Date

The goal of this program is to increase human understanding of fundamental subnuclear interactions. Work at Brookhaven pioneered the use of computer simulation and lattice techniques to study quark interactions and the confinement problem. Other ongoing projects include studies of the phase transition to quark-gluon matter at high temperatures, analytic techniques for treating Yang-Mills fields, mixing angles and quantum loop corrections in weak interactions, and jet production in hadronic interactions.

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Title of Project: Magnet Division R&D for the Superconducting Super Collider (SSC)

Persons in Charge: R. P. Shutt, C. Goodzeit, and E. Willen

Scientific and Professional Staff: M. Anerella, F. Atkinson, G. Bagley, A. Bertsche, E. Bleser, V. Buchanan, J. G. Cottingham, J. Cullen, P. Dahl, Y. Elisman, A. Feltman, R. Fernow, G. Ganetis, D. Gardner, A. Ghosh, C. Goodzeit, A. Greene, W. Harrison, R. Hogue, S. Kahn, E. Kelly, R. Le Roy, W. Mc Gahern, G. Morgan, S. Plate, I. Polk, A. Prodell, K. Robins, R. Rosenka, W. Sampson, W. Schneider, M. Shapiro, R. Shutt, J. Skaritka, A. Stevens, C. Sylvester, P. Thompson, P. Wanderer, T. Wild, and E. Willen

Scope of Work

The Magnet Division is currently engaged in an R&D program to develop magnets suitable for use in the SSC. Aspects of this program include participation in the Feasibility Study currently under way at LBL, the development, in cooperation with industry, of Nb_3Sn superconductor for possible use in the magnets, a collaboration with Clyde Taylor & colleagues at LBL on the development of a NbTi version of the magnet, and the construction of protoytpe 5 m magnets using one or both of these superconductors. The 5 m prototype magnets will provide information on several critical areas needed to develop a final design for the SSC magnet.

These areas include the development of tooling and techniques for winding coils and prestressing these coils in the iron yokes, quench propagation characteristics in the magnets, and development of instrumentation for measuring the magnetic field distribution in the magnets. Also included in the development program are magnetic field analysis of various designs, fabrication of the critical coil ends, and construction of the necessary power supply equipment needed in testing.

Goals and/or Major Results to Date

The first SSC magnet, 5 m long and 3.2 cm coil I.D., is expected to be ready for testing in June. This initial magnet will use NbTi superconductor. Later in the year, additional NbTi magnets will be constructed as well as some magnets with Nb_3Sn as the superconductor. This will mark the first time this potentially superior material will have been used to fabricate an accelerator magnet of such large length.

As the 5 m magnet program develops, the focus will shift to the design and construction of 16 m magnets, the length needed for the Reference Design A SSC. Experience gained in the 5 m program will point the way for the appropriate scientific and engineering considerations necessary for the construction of such long magnets.

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Title of Project: Cryogenic Division, High Energy Facilities

Persons in Charge: R. I. Louttit and D. P. Brown

Scientific and Professional Staff: D. P. Brown, Y. Farah, R. J. Gibbs, R. I. Louttit, A. P. Schlafke, J. H. Sondericker, and K. C. Wu

Scope of Work

The Cryogenic Division was formed in 1981 and given responsibility for all cryogenic aspects of the Colliding Beam Accelerator (CBA), both construction and R&D, and for providing helium services to the AGS experimental program. With the end of the CBA project in 1983, the emphasis has shifted to five primary areas:

1. Design of cryogenic systems for the SSC.

2. Design of cryogenic systems for a relativistic heavy ion collider (RHIC) to be proposed for construction at BNL.

3. Completion and testing of the 25 kW helium refrigerator begun for the CBA and to be used for RHIC and for system testing of strings of SSC magnets.

4. Operation of several helium refrigerators and cryogenic systems in support of the program of development of superconducting magnets for the SSC and for RHIC.

5. Measurement of heat loads of magnets and other components proposed for use in SSC and RHIC.

Provision of helium services to the AGS continues at a very low level.

Goals and/or Major Results to Date

A design, descriptive text, and cost estimate were produced for the cryogenic system for the SSC Reference Designs Report. A similar contribution was made to the RHIC proposal.

The Division has provided liaison with the manufacturer of the 25 kW refrigerator and inspection of the work, to insure compliance with the specification. Also the computer control system for the refrigerator (BNL's responsibility) has been received and tested, and software for refrigerator operation is being developed. The acceptance test for the entire system should begin early in FY 1985.

Support for magnet development involves nearly continuous running of the PAT and 7-foot Bubble Chamber refrigerators and occasional operation of the MAGCOOL system for forced flow testing of magnets in final configuration. This is expected to continue in FY 1985.

The heat load of a prototype transfer line section was measured.

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Title of Project: Relativistic Heavy Ion Collider Project

Person in Charge: R. Rau and H. Hahn

Scientific and Professional Staff: D. Barton, H. Hahn, Y. Lee, T. Ludlam, S. Ruggiero, R. Shutt, P. Thieberger, and L. Turf

Scope of Work

The Laboratory has undertaken the goal of creating a facility for relativistic heavy ion physics research with capabilities unmatched at any other institution.

The facility would consist of two colliding superconducting accelerator rings in the existing Colliding Beam Accelerator tunnel, which has a circumference of about 3.8 km. This collider will be capable of providing heavy ion collisions in the energy range from about 7 to 100 GeV/amu with luminosities from 10^{25} to 10^{27} cm^{-2} sec^{-1} for gold on gold. The energy range can be extended to lower values by operation in the internal fixed target mode with very high luminosities.

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The collider will allow operation over the entire mass range from protons to gold and possibly uranium, with equal as well as unequal species in the colliding beams. The counter rotating beams cross at six interaction points; three of these are already equipped with experimental halls. The insertion design provides 20 m of free space around the crossing point for the placement of experimental detectors. The beams are focused at the crossing points to a few millimeters and the interaction diamond length is less than 1 m.

The collider will accept and accelerate the heavy ion beams from the AGS which will become available as a result of the construction of the beam transfer tunnel linking the Alternating Gradient Synchrotron (AGS) with the existing Tandem Van de Graaff facility at Brookhaven.

Goals and/or Major Results to Date

A possible scenario for the Relativistic Heavy Ion Collider was developed and a preliminary construction proposal including cost estimate was prepared. Future work will be directed towards the development of a more detailed cost-optimized design study. A more detailed review of the beam dynamics and of performance limiting effects will be carried out. Supporting R&D work covering critical accelerator components will be initiated.

The program includes the construction and testing of prototype superconducting dipole and quadrupole magnets satisfying the specific collider requirements.

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Award No.: DE-AC02-76CH03000

Title of Project: Fermilab Theoretical Physics

Person in Charge: C. Quigg

Scientific and Professional Staff: W. Bardeen, J. Bjorken, S. Das, E. Eichten, K. Ellis, C. Hill, C. Leung, S. Love, P. Mackenzie, S. Parke, C. Quigg, S. Rao, J. Schonfeld, D. Seckel, T. Taylor, and H. Thacker

Scope of Work

The Theoretical Physics Department at Fermilab carries out basic research in various areas of theoretical elementary particle physics. Members of the Department participate regularly in meetings of the Laboratory's Physics Advisory Committee and related committees, which contribute directly to the scientific leadership of the Laboratory. A series of academic lectures on current research topics is heavily dependent upon Fermilab theorists.

The Department maintains an active program for visiting theoretical physicists. Typically, support is provided for several hundred visitors a year. In most cases the visits last for a period of a few days to a month. This vigorous program is one of Fermilab's significant contributions to the vitality of theoretical research at the participating universities.

Recent research has covered a broad spectrum of current problems in elementary particle physics ranging from formal studies of the foundations of the understanding of field theory to the anticipatory phenomenology of future accelerators.

Fermilab is developing an active program in theoretical astrophysics, which is working in close cooperatin with the program in theoretical particle physics. Recently this synergistic relation led to the Inner Space - Outer Space meeting at Fermilab attended by more than two hundred people. The astrophysics program is funded outside the high energy physics program.

Goals and/or Major Results to Date

Much effort has been devoted recently to studies of the discovery potential of new accelerators. A comprehensive exploration of the capabilities of a multi-TeV proton-proton collider has been undertaken. The results provide a reference point for the choice of machine parameters and for experiment design.

The general character of the Fermilab Theoretical Physics Program is expected to be maintained in the coming year. A steady growth of the group to 1.5 - 2 times its current size is projected, over a period of about five years. One area with potential for exploitation of Fermilab's special resources is the development of special computing hardware for the solution of problems in QCD and in beam dynamics.

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Title of Project: Electronic Detector & Bubble Chamber Experiments

Person in Charge: D. Jovanovic

Scientific and Professional Staff: B. Cox, L. Voyvodic, C. Lindenmeyer, A. Pitas, C. Kerns, and J. Upton

Scope of Work

The Physics Section supports elementary particle research performed by the Fermilab experimental physicists. Its relationship to the Fermilab physics staff is equivalent to that of a university physics department to its academic staff. The Physics Section exists to supply budgetary and technial support for all staff experimental activities at the Laboratory. Staff members participate in a wide variety of experiments performed at Fermilab and in various detector development projects. In addition, the Physics Department provides a home at Fermilab for Fermilab postdoctoral personnel and supports other miscellaneous activities such as the summer student program.

Goals and/or Major Results to Date

During FY 1984 the Physics Section supported Fermilab physicist participation in a number of activities including the operation of experiment E-605--a study of high transverse momentum production of single and dileptons, E-400--a measurement of hadronic production of charm, and E-715--a measurement of Σ-beta decay.

In addition to the support of data taking experiments, the Physics Section has had major obligations this year in preparing equipment which will be used in experiments running in FY 1985. Included among these experiments are E-705--a study of direct photon and charmonium neutrino interaction, E-690--a measurement of hadroproduction of charm, E=691--a measurement of photoproduction of charm in the Tagged Photon Beam, E-711--a study of dihadron production, and E-731--a precision measurement of η^{+-}/η^{00}.

The Physics Section is beginning to support fixed-target experiments which run in FY 1986 and beyond. Attention is being focussed on E-706--a study of direct photon production, E-665--a new deep inelastic muon scattering experiment for the new Muon Laboratory, and E-687--a new photoproduction experiment which will be positioned in the new Broad Band Photon Laboratory.

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Finally, the Physics Section is beginning to be involved in preparation for the TeV I collider experiments. Two major efforts associated with the D-Zero experiment include a uranium liquid Argon calorimetry effort and construction of muon detector proportional drift tubes. In addition to these two D-Zero efforts, other collider experiments will soon begin to have an impact. Among these are E-735--a search for evidence for quark/gluon plasmas and E-710--a study of $\bar{p}p$ elastic scattering at collider energies.

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Title of Project: Physics Research

Person in Charge: John Peoples, Jr.

Scientific and Professional Staff: D. E. Young, A. G. Ruggiero, F. E. Mills, and F. T. Cole

Scope of Work

Physics research for the investigation and development of advanced accelerator concepts is performed in a number of areas, including electron cooling, laser acceleration, and other advanced accelerator concepts.

Under a Small Business grant, design work is being carried out in collaboration with the University of Wisconsin and the National Electrostatic Corporation (NEC) for a prototype electron system to study beam cooling at high energies. If this work is successful, it will be possible to cool the accumulated antiproton core in the Accumulator down to much smaller emittance than is possible with stochastic cooling and the work thus has direct application at Fermilab. The electron beam in this case is a DC beam and very efficient recovery of the electron-beam energy after use is essential. This will also have application to a cw free-electron laser.

Theoretical conceptual studies have also been carried out in collaboration with the University of Wisconsin on the laser beatwave accelerator. In FY 1983, experimental studies of plasma density were begun at Wisconsin.

Research on simulation of nonlinear effects arising from the beam-beam interaction of colliding beams is being carried out.

Studies of medium energy antiproton rings will begin at a later time.

Goals and Major Results to Date

An emittance measurement of a 3 MeV electron beam has been completed. The goal of the work is to develop, build, and install an electron-cooling system for the Accumulator antiproton core.

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Measurements of plasma density are in progress for the laser accelerator, as well as conceptual studies leading toward a laser-acceleration experiment.

Beam-beam interactions have been simulated in computer runs, including the effects of external noise on average amplitude growth.

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Title of Project: Accelerator Operations

Person in Charge: J. R. Orr

Scientific and Professional Staff: M. Awschalom, T. Barnes, C. Bonham, H. Casebolt, S. Childress, A. Crawford, J. Crawford, C. Curtis, J. Elseth, D. Finley, J. Firebaugh, W. Fowler, R. Fuja, J. Gannon, R. Gerig, M. Harrison, G. Hodge, R. Johnson, H. Jostlein, J. Lackey, S. Lackey, E. Larson, P. Limon, J. Makara, R. Mau, C. Moore, G. Mulholland, C. Owen, R. Parry, T. Peterson, H. Pfeffer, S. Pruss, R. Rice, R. Rihel, C. Rode, C. Schmidt, J. Theilacker, E. Treadwell, R. Walker, J. Walton, and P. Yurista

Scope of Work

Accelerator Operations includes cryogenics, replacement parts, and support required for the operation of all components of the accelerator complex. This activity provides beams of protons which fit the requirements of the high energy physics program. Beams can be delivered simultaneously to the three external experimental areas and to a cancer therapy facility. The operating systems include the two 750 KeV preaccelerators, the 200 MeV Linac, the 8 GeV fast-cycling Booster Synchrotron, the 400 GeV accelerator, the superconducting Energy Saver ring, and the primary beam Extraction and Switchyard systems. Also included is a portion of the operation of the Central Helium Liquefier.

Goals and/or Major Results to Date

In March 1983, the last Energy Saver magnet was installed in the tunnel. On April 22, 1983, 150 GeV protons were injected into the Saver and successfully transported one-third of the way around the ring to a temporary beam dump. On July 4, 1983, beam was accelerated to an energy of 512 GeV in the Energy Saver for the first time. During the remainder of FY 1983 accelerator development and studies were pursued that brought the energy to 800 GeV.

During FY 1984, the Energy Saver was operated for high energy physics. At the beginning of the year, operation at 400 GeV finished experiments remaining in the 400 GeV program. During the second quarter, operation moved to approximately 800 GeV. The accelerator was turned off in the second quarter of FY 1984 to install low-beta quadrupoles in the B-Zero collision area and to construct the antiproton production targeting system near F18 and extra rf stations. The nitrogen reliquefier will also be commissioned as part of the Central Helium Liquifier complex. In FY 1985, emphasis will be on sustained operation and reliability, while increasing the energy and intensity of the superconducting accelerator.

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Title of Project: Accelerator Operations Support

Person in Charge: J. R. Orr

Scientific and Professional Staff: E. Anderson, R. Andrews, L. Bartelson, D. Beechy, G. Biallas, D. Bogert, C. Briegel, K. Cahill, L. Chapman, J. Dinkel, R. Ducar, R. Flora, A.Franck, J. Fritz, M. Glass, R. Goodwin, T. Groves, R. Hanson, G. Johnson, M. Johnson, W. Knopf, G. Krafczyk, F. Lange, G. Lee, J. Lockwood, P. Lucas, W. Marsh, D. Martin, M. Martin, P. Martin, M. May, R. McLin, H. Miller, J. Misek, S. Morris, F. Nagy, M. Palmer, S. Reeves, J. Reid, R. Reilly, J. Ryk, J. Satti, L. Sauer, T. Savord, K. Seino, M. Shea, S. Sommers, M. Storm, G. Tool, K. Ueno, A. Waller, T. Watts, D. Wildman, L. Winterowd, D. Wolff, and J. Zagel.

Scope of Work

Accelerator Operations Support includes parts and support required for the design, fabrication, installation, maintenance, repair, testing, component improvement, and other miscellany required for efficient operation of all acclerator systems including the primary proton beam switchyard systems. Operational support activities relative to accelerator systems (Preaccelerators, Linac, Booster, Main Ring, Energy Saver, including the Central Helium Liquefier, Beam Extraction, and Switchyard) are performed in close coordination with the activities of the general accelerator R&D program.

Goals and/or Major Results to Date

The major support activity was installation of Energy Saver systems and development of the controls software. Installation of all systems--magnets, refrigerators, controls, and safety systems was completed so that beam was injected into the Saver and accelerated to 512 GeV. While Energy Saver commissioning was in progress, the bulk of support activities were transferred to installation of the Switchyard to deliver beam to the high energy physics program.

The emphasis will be on high intensity, energy, reliability, and operating efficiency of this very complicated array of machines. It must be realized that with the Preaccelerator, Linear Accelerator, Booster, Main Ring, Saver/Tevatron superconducting ring, and a switchyard with up to nine primary proton beams, the Fermilab accelerator complex will require a large number of skilled people in order to make the complex operate efficiently. The commissioning and operation of the Antiproton Source complex and the attendant beam choreography will begin in FY 1986 and again, smooth, reliable, professional operation is essential for success.

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Title of Project: Antiproton Source Operation

Person in Charge: John Peoples, Jr.

Scientific and Professional Staff: Tevatron I Section and Accelerator Division Scientific and Professional Staff

Scope of Work

This work will make it possible to operate and maintain the Antiproton Source for the commissioning of the Tevatron as a proton-antiproton collider, the continuation of the R&D on stochastic cooling and antiproton production, and colliding beam physics.

The installation of the Antiproton Source, including the 120 GeV proton line, the Antiproton Target Station, the Antiproton Injection Line, Antiproton Extraction Line, and Debuncher and Accumulator, will be completed during the second quarter of FY 1985. After the completion of electrical power tests and the initial phase of beam tests, the project personnel working on the Antiproton Source will be reorganized in order to shift the effort from fabrication and installation to commissioning and maintenance. An Antiproton Source Department will be established within the Tevatron I Section to maintain and operate the recently completed accelerator subsystems. The work here will make it possible to operate the Antiproton Source starting in FY 1985 as part of the colliding beams program at Fermilab. Since the operation of the Antiproton Source is not part of the scope of the Tevatron I project, separate funds are required for that purpose.

Goals and/or Major Results to Date

The Antiproton Source Department will operate the Debuncher, Accumulator, Target, and beam lines for the development of targeting and stochastic cooling methods and systems and will make improvements in the Antiproton Source system to increase its performance and reliability. Operation will be turned over to the Accelerator Division Operations Department as colliding beam operation becomes more routine.

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Title of Project: Fermilab Experimental Areas Operations

Person in Charge: R. Dixon

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Scientific and Professional Staff: W. Baker, J. Becker, F. Bellinger, L. Beverly, G. Book, N. Bosek, C. Brown, D. Burke, S. Butala, J. Butler, J. Bywater, D. Carey, H. Carter, R. Coleman, D. Cosgrove, J. Cossairt, R. Currier, P. Czarapata, K. Dixon, R. Dixon, R. Drysdale, D. Eartly, H. Fenker, M. Frohne, P. Garbincius, M. Gerardi, A. Glowacki, D. Green, H. Haggerty, P. Hall, S. Hansenn, J. Hawkins, W. Higgins, A. Jonckheere, G. Koizumi, K. Krempetz, L. Kula, J. Lach, E. LaVallie, J. Lindberg, A. Malensek, G. Miller, J. Morfin. M. Mugge, T. Murphy, S. Orr, A. Passi, S. Pordes, R. Schailey, W. Smart, S. Sobczynski, R. Sood, W. Spalding, R. Stanek, R. Stefanski, S. Stoy, H. Stredde, B. Strickland, L. Studde, G. Tassotto, R. Tokarek, R. Trendler, E. Villegas, A. Visser, H. White, J. Wooden, and C. Worel

Scope of Work

The recent formation of the new Experimental Areas Department (EAD) at Fermilab has succeeded in its goal of unifying operating methods and systems for the three main fixed-target experimental areas--Meson, Neutrino, and Proton--each with its distinctive physics focus and operational problems.

Primary proton beams from the accelerator are transported to each of the three experimental areas where they are further split and targeted to create three to four primary, secondary, or tertiary particle beams directed into specific experimental halls. Many of these beams use superconducting magnets. In each of the final beamlines there are typically two experiments either being assembled, taking data, being modified, or being dismantled.

When the Tevatron II project is complete, this array of beams will include several high energy, high intensity hadron beams and two photon beams, a polarized proton beam, a muon beam, both a conventional and prompt neutrino beam, and several flexible test beams. EAD also operates a number of facilities including the Tagged Photon Spectrometer, the Multiparticle Spectrometer, two large neutrino detectors, and the fifteen foot bubble chamber.

Goals and/or Major Results to Date

EAD resumed operation for high energy experiments in the fall of 1983 when the Energy Saver started operation. By that time, many of the primary and secondary beams, as well as some of the experimental areas, had been rebuilt and upgraded. During the fall 1983 running period, the beam energy was held at 400 GeV in order to complete two existing experiments. In early 1984, the beam energy was raised to 800 GeV to begin exploiting the full power of the Tevatron.

Goals for the next three years include completion of the new muon and broad band photon beams, the polarized proton beam, and the prompt neutrino beam as well as implementation of a number of significant new experimental facilities.

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Title of Project: Fermilab Collider Detector Department

Persons in Charge: R. Schwitters and A. Tollestrup

Scientific and Professional Staff: M. Atac, E. Barostti, M. Binkley, M. Bowden, D. Carlson, J. Carroll, T. Collins, C. Day, G. Drake, T. Droege, J. Elias, J. Grimson, M. Haldeman, D. Hanssen, B. Haynes, M. Henry, H. Jensen, R. Kadel, H. Kautzky, R. Kepart, M. Larwill, M. Leininger, J. Marsh, C. Nelson, C. Newman-Holmes, J. O'Meara, D. Quarrie, C. Rotolo, S. Segler, W. Stuermer, C. Swoboda, D. Theriot, A. Tollestrup, K. Turner, R. Vidal, R. Wagner, R. Yamada, and J. Yoh

Scope of Work

This activity supports accelerator operations in the B0 Colliding Beams Experimental Area at Fermilab, installation of the Collider Detector at Fermilab (CDF), and experimental operations related to the CDF detector. Initial activities involve preparation of the B0 area for accelerator operations and detector installation. Following the installation of CDF, the activities will shift to detector operations, experimental running, and improvements to CDF.

The collider detector is a large general purpose detector system designed to explore the physics of 2 TeV proton-antiproton collisions made possible by the Tevatron I project. The design and construction of the detector is being carried out by a Fermilab-led consortium of physicists from ten U.S. universities (Brandeis University, University of Chicago, Harvard University, University of Illinois, University of Pennsylvania, Purdue University, Rockefeller University, Rutgers University, Texas A&M University, and University of Wisconsin), three U.S. National Laboratories (Argonne, Fermilab, Lawrence Berkeley), and several institutions in Japan and Italy. The major elements of the detector include a superconducting solenoid magnet with associated satellite refrigerators, the central tracking chambers, the forward tracking chambers, the hadron and electromagnetic calorimeters, the muon chambers, the front-end electronics, and the data acquisition electronics.

Goals and/or Major Results to Date

Construction of the B0 Colliding Beams Experimental Area was completed in the latter half of 1983. The low-beta quadrupoles have now been installed and operated. The superconducting coil for the solenoid magnet will be tested in the latter half of 1984. A preliminary test run using a partially completed detector will take place in the latter half of 1985.

The culmination of many years of effort will occur in 1986. The construction of the Main Ring overpass at B0 will be completed so that normal data taking operations of CDF can begin with close to the full complement of hardware.

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FERMI NATIONAL ACCELERATOR LABORATORY
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Title of Project: Fermilab Research Services Operations

Person in Charge: F. Beck

Scientific and Professional Staff: D. Anderson, J. Bartlett, A. Baumbaugh, E. Bosworth, W. Craddock, R. Dachniwskyj, R. Fast, J. Fitch, H. Hart, A. Ito, J. Kelly, B. Kramper, T. Lahey, A. Lynch, B. Mackinnon, S. Majewski, H. Montgomery, R. Sanders, J. Simanton, R. Smith, J. Stoffel, M. Stone, R. Wands, C. Wegner, R. West, W. Yang, R. Yarema, and T. Zimmerman

Scope of Work

The Fermilab Research Services Department provides extensive support to the experimental program of the Laboratory. These services include operations, maintenance, construction, and development associated with the program. Some of the Research Services activities include the following operations.

1. Fabrication and operation of liquid hydrogen targets.
2. Fabrication and testing of analysis and beamline magnets of both the conventional and superconducting type.
3. Operation of a magnetic field measurement facility.
4. Construction, operation, and maintenance of beam monitor and control systems including both software and hardware activities, primarily in the external beamline but extending also to Main Ring and Tevatron monitoring and control.
5. Survey and alignment services for both the Accelerator and Research Division.
6. Operation of a facility for prototype printed circuit fabrication and production of large PC boards for detector construction.
7. Provision of engineering design and construction (electronic and mechanical) for special experimental detector needs.

Ten of the eleven groups which constitute the Research Services Department participate in these activities. The eleventh group, Detector R&D, was formed only recently and is just beginning to function; it has no operational responsibilities.

Goals and/or Major Results to Date

The Research Services Department has been responsible for many activities involved in the smooth transition to operation of the Tevatron for physics. As an example, the hardware associated with the revised beam control system has proven to be exceptionally reliable during the first Saver running period.

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Research Services goals include the development of several large magnets as well as associated refrigeration systems. These magnets include several conventional magnets for experiments, the prompt beam dump magnets, as well as the Tohoku bubble chamber and the CDF coil.

Goals for controls include the development of software for smoother experimental area and beamline operations.

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Title of Project: General Computing Operations

Person in Charge: A. Brenner

Scientific and Professional Staff: S. Ahlgrim, J. Appel, G. Bellendir, D. Berg, A. Brenner, R. Bunker, D. Burch, C. Canada, P. Constanta-Fanourakis, C. DeBaun, E. Denito, K. Eng, R. Forster, S. Gannon, P. Heincke, J. M. Ingebretsen, J. O. Ingebretsen, H. Johnstad, A. Kreymer, E. Kuhaitis, J. Lacher, A. Lambert, A. Lubinsky, J. Mack, A. Neubauer, J. Nicholls, T. Nicinski, P. Perkins, J. Pfister, R. Pordes, M. Pyatetsky, E. Quigg, D. Ritchie, D. Sachs, R. Thatcher, R. Thompson, and V. White

Scope of Work

The Computing Department at Fermilab is responsible for the Laboratory's general computing, fast electronics, data acquisition computing, and related operations. These encompass the following activities.

1. Fast turnaround computing for the support of experiments taking data.
2. Batch processing for the analysis of a major quantity of the data acquired in the experiments at Fermilab and theoretical physics computations by Fermilab theorists. These first two tasks are supported by a powerful, loosely coupled system of Cybers. These are operated 24 hours a day, 7 days a week.
3. Minicomputer system support including on-line data acquisition, hardware maintenance, and software development. This activity supports some sixty minicomputers and a dozen mid-size computers.
4. Provision of interactive facilities for preparation of code.
5. Support of business computing hardware and some elements of the related software.
6. Support of some of the engineering and computer-aided design efforts at the Laboratory.
7. Maintenance of the Physics Research Equipment Pool (PREP) of electronics modules.

8. Repair throughout Fermilab of all standard PREP instruments and other electronic Laboratory equipment.

A serious effort is made to coordinate the development of these resources with the evolving needs of the physics program. Recently a high level ad hoc committee with a range of membership from the high energy physics and computing science communities was appointed to help coordinate these needs.

Goals and/or Major Results to Date

The computing load at the Laboratory has grown steadily over the years. Improvements in performance and certain efficiences have kept the service level adequate for the needs. A major simplification was the early standardization on a minicomputer system and the development of a flexible minicomputer software called MULTI.

Goals include an acceleration in the rate at which the Laboratory is providing interactive computing, networking, and super minicomputers. A second Cyber 875 CPU will be installed to bring the computing capacity to seven Cyber 175 equivalents.

For the second half of the eighties a major new architecture acquisition will be acquired. In addition, a new separate computing facility building has been requested. These facilities are needed to cope with an expected demand rise of ten to a hundred.

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Title of Project: General Accelerator R&D

Person in Charge: J. R. Orr

Scientific and Professional Staff: C. Ankenbrandt, S. Bristol, A. Crawford, J. Fitzgerald, Q. Kerns, M. May, K. Meisner, W. Merz, S. Ohnuma, F. Turkot, and R. Webber

Scope of Work

The accelerator R&D program is devoted to understanding and improving the operating characteristics of all of the accelerator systems at Fermilab in order to increase their reliability and to improve the beam intensity and quality. The basic strategy underlying the program is to concentrate resources in those areas where improvements appear most promising and will result in achieving the goals of the physics research program. The programmatic emphasis shifts periodically as the success of a particular improvement project in one accelerator system illuminates the limitation imposed by deficiencies in other systems.

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Included in this program are development of special devices and systems for extraction of the proton beam from the Energy Saver, transport and splitting of this beam in the Switchyard, and targeting of the beam in the internal and external experimental areas. Also included after FY 1985 will be the similar special devices and systems for extraction of the proton beam from the Main Ring for production of antiprotons and reinjection of antiprotons into the Main Ring.

Goals and/or Major Results to Date

A myriad of developments in refrigeration, power systems, safety systems, controls, etc., along with the tremendous developments in the controls system, were the most noteworthy activities involved in bringing the Saver into commission as an operating accelerator.

Effort will be focused on preparations for implementing the antiproton option and improving the quality and intensity of beams for the fixed-target program.

In FY 1985 a mini-overpass will be installed as a test in the B0 straight section. This is the first time such a distorted orbit has been installed in a working accelerator. Based on the results of these experiments, preparations will be made to install a full overpass in B0.

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Title of Project: SSC Research and Development

Person in Charge: J. R. Orr and R. A. Lundy

Scientific and Professional Staff: J. Carson, H. Edwards, E. Fisk, W. Fowler, N. Gelfand, R. Hanft, P. Limon, P. Mantsch, A. McInturff, L. Michelotti, W. Ng, T. Nicol, R. Neimann, C. Rode, A. Russell, E. Schmidt, T. Toohig, and G. Tool

Scope of Work

This program includes materials and supplies necessary to support the R&D activities required to develop a viable systems design for a 20 TeV-on 20 TeV Superconducting Super Collider. Initial work will concentrate on magnet development including superconducting cable and production tooling. This will evolve to development of the various subsystems required for such an accelerator. In later stages, systems development will be carried out involving a test string of magnets with all of its associated systems.

Goals and/or Major Results to Date

A major goal for the FY 1984 SSC Research and Development program is to develop an inexpensive 4.5 to 5T dipole suitable for a 20 TeV/beam collider. A critical first step is to construct and test a series of

2 foot long model superconducting dipoles in order to evaluate and optimize methods of collared coil construction.

In conjunction with industry, a developmental program leading to a more cost-effective superconductor will be implemented.

The design of the accelerator itself will also begin. Conceptual cryogenic designs will be done and will include computer simulation studies to predict the performance of the cryogenic system.

Goals include the design and development of tooling for a pilot development of quadrupoles and trim magnet packages and the design and quench propagation will be carried out to find better quench protection methods for large intermediate field magnets.

Cryogenic design and computer simulation and development for a prototype refrigerator will also be carried out.

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Title of Project: Research and Development in Support of the Tevatron I Project

Person in Charge: John Peoples, Jr.

Scientific and Professional Staff: Tevatron I Section and Accelerator Division Scientific and Professional Staff

Scope of Work

The purpose of the Tevatron I Project is to provide a source of antiprotons to the Tevatron Ring for colliding-beam experiments. As part of the project, an antiproton production target, focusing lenses, beam lines, and Debuncher and Accumulator storage rings will be built.

The construction and installation of the Accumulator components and the construction and the installation of some of the beam line components are part of the R&D in support of Tevatron I. The construction and installation of the Debuncher components, except for the stochastic cooling prototypes, and the remainder of the beam line components are part of the construction funded part of the Tevatron I project. The fabrication of all prototype components is included in the R&D in support of the Tevatron I project.

Goals and/or Major Results to Date

A magnet prototype program has been initiated and has resulted in successful designs for the several types of dipole and quadrupole magnets. Prototype programs of rf cavities, stochastic cooling equipment, and electronic kickers and supplies is in progress. Successful lithium focusing lenses have been built and later versions are now being built. The goal of the R&D is to provide components meeting specifications for the Antiproton Source and a test bed for stochastic cooling development.

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Title of Project: Advanced Accelerator R&D

Person in Charge: J. R. Orr

Scientific and Professional Staff: D. Edwards, N. Gelfand, R. Johnson, K. Koepke, L. Michelotti, W. Ng, A. Russell, S. Snowdon, L. Teng, and A. Van Ginneken

Scope of Work

The Advanced Accelerator R&D program includes materials, supplies, and support for the investigation of advanced accelerator concepts.

Goals and/or Major Results to Date

The low-beta insertion for the B0 interaction area will be installed and commissioned. Research will include beam orbit studies using the accelerator as a test bed combined with orbit simulation work on the computer, as well as development of better instrumentation for beam monitoring and control. A second low-beta insertion for D0 will be designed. Higher gradient quadrupole designs for low-beta will be developed.

A program will begin to improve the properties (e.g. emittance) of the proton beam. This program will lead to more intense secondary beams for the fixed-target program and higher luminosity in the collider.

Intensive research and development must be conducted on the Main Ring injector in order to improve its performance after the construction of the overpasses at the B0 and D0 straight sections. Research and development will also continue on methods of improving the Tevatron magnets in order to reach higher energies.

Systems will be developed as needed to improve the lifetime of stored beam in the Tevatron and to prevent beam losses leading to downtime from magnet quenches.

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Title of Project: Fermilab Experimental Area Beam and Device R&D

Person in Charge: R. Dixon

Scientific and Professional Staff: W. Baker, J. Becker, F. Bellinger, L. Beverly, G. Book, N. Bosek, C. Brown, D. Burke, S. Butala, J. Butler,

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J. Bywater, D. Carey, H. Carter, R. Coleman, D. Cosgrove, J. Cossairt, R. Currier, P. Czarapata, K. Dixon, R. Dixon, R. Drysdale, D. Eartly, H. Fenker, M. Frohne, P. Garbincius, M. Gerardi, A. Glowacki, D. Green, H. Haggerty, P. Hall, S. Hansen, J. Hawkins, W. Higgins, A. Jonckheere, G. Koizumi, K. Krempetz, L. Kula, J. Lach, E. LaVallie, J. Lindberg, A. Malensek, G. Miller, J. Morfin, M. Mugge, T. Murphy, S. Orr, A. Passi, S. Pordes, R. Schailey, W. Smart, S. Sobczynski, R. Sood, W. Spalding, R. Stanek, R. Stefanski, S. Stoy, H. Stredde, B. Strickland, L. Studde, G. Tassotto, R. Tokarek, R. Trendler, E. Villegas, A. Visser, H. White, J. Wooden, and C. Worel

Scope of Work

The Fermilab Experimental Areas Department (EAD) research and development work includes beam transport design, conventional and superconducting magnetic transport element development, beamline control improvement, and primary and secondary targeting systems development. Among general developments necessary for most beamlines are new power supply regulators with improved stability, a remote high current polarity reversing switch, and a way of fast-ramping magnets to serve multiple users during a single spill. The higher energy and intensity of the particle beams produced by the Tevatron have necessitated a careful optimization and redesign of many aspects of the beam transport and targeting systems in the experimental area.

Research and development is also necessary for the detector facilities operated by EAD. For example, the advent of holographic bubble chamber optics in the 15 foot and 1 meter bubble chambers has necessitated the development of laser-based illumination systems for these chambers. Various auxiliary muon and hadron tagging systems based on proportional and scintillation counter techniques are also needed for the bubble chamber systems.

Goals and/or Major Results to Date

First operation of the Tevatron has required significant new developments in beam elements and the associated power supplies and cryogenics as well as beam monitoring and detector upgrading. The initial operation of the experimental areas with these new developments has been quite successful. Future goals include development of quadrupole and snake dipole magnets for the polarized proton beams, laser pulse stretchers for bubble chamber holography, and improved interlock and control systems.

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Title of Project: Collider Detector Research and Development

Persons in Charge: Schwitters and A. Tollestrup

Scientific and Professional Staff: M. Atac, E. Barsotti, M. Binkley, M. Bowden, D. Carlson, J. Carroll, T. Collins, D. Day, G. Drake,

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T. Droege, J. Elias, J. Grimson, M. Haldeman, D. Hanssen, B. Haynes, M. Henry, H. Jensen, R. Kadel, H. Kautzky, R. Kephart, M. Larwill, M. Leininger, J. Marsh, C. Nelson, C. Newman-Holmes, J. O'Meara, D. Quarrie, C. Rotolo, S. Segler, W. Stuermer, C. Swoboda, D. Theriot, A. Tollestrup, K. Turner, R. Vidal, R. Wagner, R. Yamada, and J. Yoh

Scope of Work

A substantial amount of R&D effort has been required in connection with the Collider Detector at Fermilab in order to determine which detector types best meet the physics needs, to optimize the performance of the detectors while keeping the costs down, and to find ways to produce the needed quantities reliably and cost effectively. This R&D work has been an on-going effort throughout the construction phase of the project because the detector is being built in a phased manner.

Goals and/or Major Results to Date

Some of the important R&D achievements include the magnet design, development of the tracking chambers, invention of the Rabbit electronic system for an analog bus, and development of a trigger supervisor system.

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Title of Project: Fermilab Particle Detector Research and Development

Person in Charge: F. Beck

Scientific and Professional Staff: D. Anderson, J. Bartlett, A. Baumbaugh, E. Bosworth, W. Craddock, R. Dachniwskyj, R. Fast, J. Fitch, H. Hart, A. Ito, J. Kelly, B. Kramper, T. Lahey, A. Lynch, B. Mackinnon, S. Majewski, H. Montgomery, R. Sanders, J. Simonton, R. Smith, J. Stoffel, M. Stone, R. Wands, C. Wegner, R. West, W. Yang, R. Yarema, and T. Zimmerman

Scope of Work

The Fermilab Research Division and particularly the Research Services Department are responsible for research and development work aimed at producing improved particle detection devices for use in high energy physics experiments, including future colliding beams facilities. A Particle Detector Group has been formed recently which will be involved in the conception and development of new particle detection methods and devices.

An adjunct to detector development is detector electronics. Examples include a readout system for an active target/high resolution vertex detector and a "Cluster Finder" to process the analogue signals from a rectangular array of 400 scintillation glass counters. Some of the R&D effort is also devoted to development of improved diagnostic devices and control systems for secondary beamlines.

Development work on conductor types and production techniques for specialized magnets is also included. Examples include selecting the conductor and establishing the coil winding technique for the Prompt Neutrino beam dump magnets and the exploration of ultrasonic techniques to measure the quality of solder bonds in superconducting coils.

Goals and/or Major Results to Date

The research of the new Particle Detector Group will initially be directed toward ring imaging Cerenkov counters. Other potential areas of interest include BaF_2 and neutron detection. There will also likely be efforts in fast timing, liquid ionization detectors, and detectors with high spatial resolution and good two-particle separation. It is expected that this group will mature into a center of excellence for particle detector R&D.

In general, future R&D will be devoted to the support of later stage Tevatron II experiments. In addition some R&D work will be carried out for the D0 Detector.

In the controls area R&D work will be directed toward integrating computer monitoring and control of all of the cryogenic refrigeration systems in the experimental areas into the normal control system.

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Title of Project: Fermilab Data Handling Research and Development

Person in Charge: A. Brenner

Scientific and Professional Staff: S. Ahlgrim, J. Appel. G. Bellendir, D. Berg, A. Brenner, R. Bunker, D. Burch, C. Canada, P. Constanta-Fanourakis, C. DeBaun, E. Dentino, K. Eng, R. Forster, S. Gannon, P. Heincke, J. M. Ingebretsen, J. O. Ingebretsen, H. Johnstad, A. Kreymer, E., Kubaitis, J. Lacher, A. Lambert, A. Lubinsky, J. Mack, A. Neubauer, J. Nicholls, T. Nicinski, P. Perkins, J. Pfister, R. Pordes, M. Pyatetsky, E. Quigg, D. Ritchie, D. Sachs, R. Thatcher, R. Thompson, and V. White

Scope of Work

The Data Handling R&D activities are aimed at improving the capability of data acquisition, multicomputer interaction, and data analysis facilities at Fermilab. The development of some FASTBUS components, software enhancement, and graphics development are also included.

An example of these activities is a project to couple multiple CPU's for operating experiments. The first experiments, in fact, chose from two classes of architectures using PDP-11's and VAX computers. Software development projects include system design effort for cryogenic controls, TV displays of experimental areas targeting pulse-by-pulse, a VAX device independent graphics (DIGS) hardcopy capability, a disk logging capability

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in RT/MULTI, and the first distributable VMS drivers for the coupled machine DR11W and the FASTBUS UPI. Extensions of existing MULTI/DA concepts to interface with FASTBUS systems (e.g., a FASTBUS Diagnostic Language modeled after CAMAC Diagnostic Language) are also being developed.

Hardware projects include a major effort to add supportable components for trigger processing modules and development work related to new computer-controlled high voltage systems and new FASTBUS TDC prototypes.

Goals and/or Major Results to Date

The next Tevatron-era experiments will be considerably larger and more complex than most of the current experiments and will require more sophisticated on-line computation. Increased emphasis on 32-bit machines and added systems capability for new software products will be important. Substantial additional work is planned on networking and graphical interactive computing techniques.

New devices and preprocessors are expected to become major components in data acquisition systems. This will require the development of appropriate levels of systems software and user application software.

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Title of Project: Fermilab Advanced Computer Research and Development

Person in Charge: T. Nash

Scientific and Professional Staff: V. Areti, G. Case, M. Fischler, I. Gaines, D. Husby, and T. Nash

Scope of Work

The objective of the Advanced Computer Research and Development Program (ACP) is to study the compute-bound problems of high energy physics. This field has outgrown the capabilities that can be provided at reasonable cost by commercially available computing systems. The resulting computing crunch is a severe impediment to physics progress in three diverse areas: experiment event reconstruction, accelerator orbit studies, and lattice gauge calculations.

Several recent developments have made possible new approaches to computing. The existence of powerful 16 and 32 bit commercial microprocessors with efficient FORTRAN compilers allows the construction of extremely cost-effective computing engines assembled from large numbers of these devices. Advances in very large scale integration and memory technology make it reasonable to consider dedicated special purpose hardware built as adjuncts to microprocessor modes. By restricting attention to a finite (but large) class of problems with natural trivial parallelism one can expect to design and commission on a short time scale a system of 100-200 nodes based on a simple, loosely coupled architecture.

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The Fermilab ACP Flexible Multiprocessor project is a modular, loosely coupled array of commercial microprocessors with special-purpose hardware devices which is initially targeted at the major computing-intensive problems of high energy physics. The results are expected to have further applications to a large range of computing-intensive problems.

Goals and/or Major Results to Date

The project will provide computing that is substantially greater than an order of magnitude more cost effective than current commercial CPUs. The goal for the initial reconstruction processor is to build a system with the computing power of ten Cyber 175s for less than $500K. This system will initially consist of roughly one hundred processing nodes controlled by a minicomputer host. Later, attached special-purpose hardware co-processors will be added to provide even greater processing power to meet the goals. Ultimately the system will be tested as a real time high level trigger for CDF or another high-data-rate experiment.

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Award No.: DE-AC03-76SF00098

Title of Project: The Time Projection Chamber (TPC)

Person in Charge: P. Oddone

Scientific and Professional Staff: M. Alston-Garnjost, A. Barbaro-Galtieri, A. V. Barnes, A. Bross, O. Chamberlain, A. R. Clark, O. I. Dahl, C. Day, P. H. Eberhard, B. Gabioud, W. Hofmann, S. Kaye, R. W. Kenney, L. T. Kerth, R. Kofler, S. C. Loken, G. R. Lynch, R. J. Madaras, J. N. Marx, P. Nemethy, D. R. Nygren, P. J. Oddone, M. Pripstein, P. Robrish, M. T. Ronan, R. R. Ross, R. Sauerwein, M. L. Stevenson, E. Wang, R. Avery, K. A. Derby, T. Edberg, J. W. Gary, H. Huth, W. Moses, F. R. Rouse, M. D. Shapiro, R. Van Tyen, and Z. Wolf

Scope of Work; Goals and/or Major Results to Date

The PEP-4 Experiment is a collaborative effort with participants from LBL, UCLA, UCR, Johns Hopkins University, Yale University, University of Massachusetts and University of Tokyo. The experiment uses a comprehensive detector which has as its core the Time Projection Chamber developed at LBL. It shares Interaction Region 2 with the Two Gamma Detector, PEP-9, with which it is highly integrated. PEP-4 has collected so far approximately 80 inverse picobarns of data. The data are unique in their comprehensive particle identification. Results include the best limits on the production of fractionally charged particles (2/3e and 4/3e), the most extensive data on charged particle ratios and differential cross sections, the only pi-zero production data from PEP, baryon-antibaryon correlations which already have ruled out models, the only detected phi signal in either PEP or PETRA, and associated with this the best data on vector meson production, a study of polarization produced in fragmentation, a search for as yet undetected charmed mesons such as the F^*, a study of particle composition of tagged jets such as charm and beauty jets, a study of particle composition for gluon jets, the cleanest fragmentation functions for beauty jets derived from direct electron and muon signals. Approximately 12 Ph.D. theses will be completed during 1984 at Berkeley and elsewhere. In addition to the above data on annihilation events, the group collaborates with the Two Gamma Experiment, PEP-9, in nearly all two photon physics. Results so far include the study of two, four, and multi-body final states using the particle identification properties of the TPC and the comprehensive photon detection of both detectors, the study of large p_t jets produced in two photon events, the determination of the structure functions of the photon, and the search for expected and unexpected resonances.

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Title of Project: The Mark II Detector

Persons in Charge: G. Goldhaber and G. H. Trilling

Scientific and Professional Staff: G. S. Abrams, G. Gidal, G. Goldhaber, J. Haggerty, D. A. Herrup, J. A. Kadyk, G. H. Trilling, A. R. Baden, J. H. Boyer, F. E. Butler, M. S. Gold, I. Juricic, M. E. Nelson, W. B. Schmidke, P. D. Sheldon, D. Wood, and C. de la Vaissiere

Scope of Work; Goals and/or Major Results to Date

The Mark II detector is operated at the PEP storage ring in collaboration with the SLAC Groups C and E and with a Harvard University group. A total integrated luminosity of about 223 pb^{-1} has been collected so far. The high resolution vertex drift chamber has continued to operate well and has played an essential role in much of the physics analysis from these data. Recent results from the Mark II data have included the world's most precise measurement of the τ lepton lifetime, the first measurement (simultaneously with the MAC group) of the b quark lifetime, further tests of electroweak theory through charge asymmetry measurements in dilepton and di-b-quark final states, improved measurements of the D^0 lifetime, improved studies of the b quark fragmentation function into B-mesons, new lower bounds for the mass of the hypothesized selectron, and the scalar supersymmetric partner of the electron.

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Title of Project: CDF Project at Fermilab

Person in Charge: W. Carithers

Scientific and Professional Staff: W. Carithers, W. Chinowsky, R. Ely, M. Franklin, and J. Siegrist

Scope of Work; Goals and/or Major Results to Date

LBL physicists are collaborating with Fermilab and twelve other institutions throughout the world on the Collider Detector at Fermilab (CDF), a device to exploit the proton-antiproton collisions of 2 TeV total energy produced by Tevatron I. The LBL group is responsible for the construction and instrumentation of the fine-grained, end-plug hadronic calorimeters. These calorimeters consist of truncated hollow cones of inner and outer half-angles of approximately 10^o and 30^o, respectively, made of alternate layers of steel and proportional tube chambers to provide sampling of the hadronic energy flow. The granularity of the calorimeters is approximately $\Delta\phi = 5^o$ in azimuth.

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At present, construction of the 520 proportional tube chambers is progressing smoothly, with completion projected by late 1984 or early 1985. In the spring of 1984, one twelfth of the full system was installed in a test beam at Fermilab for calibration. It is projected that the CDF will receive a very brief test run of $\bar{p}p$ collisions in mid-1985, with the actual commissioning of the Tevatron I and the beginning of data taking in the first half of 1986.

The LBL group has recently accepted additional responsibility for the TDC data acquisition electronics for input via FASTBUS to the host computer. This effort involves R&D on the readout processor system.

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Title of Project: Search for the Effects of a Right-handed Gauge Boson

Person in Charge: M. Strovink

Scientific and Professional Staff: J. Carr, G. Gidal, K. Shinsky (deceased), H. Steiner, M. Strovink, R. D. Tripp, B. Balke, A. Jodidio, and D. Stoker

Scope of Work; Goals and/or Major Results to Date

The search for the effects of a right-handed gauge boson in μ^+ decay, by means of a precise measurement of the polarization parameter ξ, was completed in 1984. Preliminary results were published in Physical Review Letters in 1983. For no mixing of W_L and W_R bosons, the preliminary limit reached was $M(W_R) > 450$ GeV. This is already the primary experimental constraint on right-handed gauge bosons coupling to Dirac neutrinos. The experiment was performed at the TRIUMF cyclotron in Vancouver, Canada in collaboration with B. Gobbi (Northwestern) and C. J. Oram (TRIUMF). The same collaboration using the same Muon Polarimeter was approved to measure the asymmetry parameter δ in μ^+ decay. The prediction $\delta = 3/4$ is embedded in a very large subset of possible weak-interaction models; experimental departure from this predicted value would have far-reaching consequences. The program in progress is the completion of data acquisition for the ξ and δ experiments at TRIUMF and continued analysis of these data, leading to publication of final results on ξ by two different methods and for δ.

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Title of Project: Theoretical Physics

Person in Charge: J. D. Jackson

Scientific and Professional Staff: O. Alvarez, K. Bardakci, P. Binetruy, R. Cahn, D. Caldi, M. Chanowitz, G. Chew, S. Dawson, M. K. Gaillard, M. Halpern, I. Hinchliffe, J. D. Jackson, S. Mandelstam, N. Snyderman, H. Stapp, T. Sterling, M. Suzuki, B. Zumino, G. Batrouni, V. Elser, R. Ingermanson, D. Issler, M. Levinson, S. Mahajan, S. Sharpe, and A. Smith

Scope of Work; Goals and/or Major Results to Date

The research of the Theoretical Particle Physics Group ranges from highly theoretical subjects, such as supergravity, to phenomenological study directly related to ongoing experiments. Though there is a substantial overlapping, most of the work falls into one of five areas: (1) Supersymmetry and Supergravity, (2) Particle Physics and Cosmology, (3) Nonperturbative Field Theory, (4) Electroweak Theory, and (5) General Phenomenology. Members of the Theory Group participate in workshops, both at LBL and elsewhere, dedicated to future machines and detectors in high energy physics. LBL theorists regularly consult with experimenters on ongoing experimental research work and with physicists in the Particle Data Group.

1. Supersymmetry and Supergravity

   A careful study was made to examine a constraint on the top quark mass in a class of such supersymmetric models. A comprehensive work on production and decay of supersymmetric particles and constraints on their masses is also being made. The effect of chiral and gravitational anomalies is examined in theories of the Kaluza-Klein type. The local Cremmer-Julia symmetry in superstring models is studied from the viewpoint of hidden symmetries.

2. Particle Physics and Cosmology

   Particle physics in the early universe is a subject of ongoing work.

3. Nonperturbative Field Theory

   Even now perturbation theory is often the only method to obtain quantitatively accurate solutions to field theory. Much effort continues to gain an insight into nonperturbative aspects of field theory.

4. Electroweak Theory

   Physical consequences of heavy Higgs bosons have been studied in production through hadron-hadron collision, a Higgs-Higgs bound state, and other aspects when the Higgs boson mass is from a half

TeV to 1 TeV. As further tests of the standard theory at and above 100 GeV, single, two- and multi-W productions have been examined in the super-high energy region.

More speculative attempts are in progress, aiming at replacement of the Higgs sector by something different from technicolors.

5. General Phenomenology

The Theory Group continues to direct much of its research effort towards problems of direct interest to experimenters, especially at LBL. Study on glueballs, $q\bar{q}$-glue states (named meiktons), and $qq\bar{q}\bar{q}$ states, with which some already existing resonances might be identifiable, is still going on. $F(c\bar{q};\ ^1S_0)$ and $F^*(c\bar{q};\ ^3S_1)$, long distance QCD through quark fragmentation and hadron correlations in rapidity plot, and prompt electrons are a few examples of the subjects of prime interest to the TPC Group.

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Title of Project: Particle Data Group

Person in Charge: T. G. Trippe

Scientific and Professional Staff: R. N. Cahn, G. Gidal, B. Levine, A. Rittenberg, T. G. Trippe, C. G. Wohl, and G. P. Yost

Scope of Work; Goals and/or Major Results to Date

The Particle Data Group (PDG) compiles high energy physics data and makes it available to the physics community, both through periodic publications such as the Review of Particle Properties, and through computer searchable data bases. PDG work is done in collaboration with a large number of institutions, among which are CERN, Durham, Helsinki, Serpukhov, and SLAC. Some members of the PDG are also active in research projects at LBL and elsewhere.

There are five major activities:

1. Compilation and publication of the "Review of Particle Properties" (RPP, LBL-100), with the associated Data Booklet and Pocket Diary.
2. Compilation of information on experiments. Publication of "Current Experiments in Elementary Particle Physics" (LBL-91) and "Major Detectors in Elementary Particle Physics" (LBL-91 Supplement).
3. Compilation and publication of information on published articles and preprints containing new data (LBL-90).

4. Interactive distribution of the compiled information described above via the SLAC SPIRES system.

5. Participation in various research projects in collaboration with LBL and other research groups.

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Title of Project: High Energy Astrophysics

Persons in Charge: (1) R. Muller and (2) G. F. Smoot

Scientific and Professional Staff: (1) F. Crawford, D. Morris, R. Muller, C. Pennypacker, P. Tans, K. Bertsche, S. Burns, P. Friedman, J. Kare, D. Lashof, S. Perlmutter, and R. Williams; and (2) G. De Amici, P. Lubin, G. F. Smoot, G. Epstein, S. Friedman, S. Levin, and C. Witebsky

Scope of Work; Goals and/or Major Results to Date

1. High Energy Astrophysics and Interdisciplinary Experiments

Experiments are being performed to study particle physics phenomena, especially in the astrophysical regime. Related projects which require the techniques of high energy and nuclear physics are also studied. Present projects include study of supernova explosions, investigations of astrophysical models for catastrophic events on the earth, development of accelerator methods for radioisotope detection, and tests of General Relativity.

2. Cosmic Background Radiation/Primordial Blackbody Radiation

The experimental program to detect anisotropies in the Cosmic Background Radiation (CBR) has continued. An anisotropy at the 10^{-3} level has been measured using a 9 mm wavelength radiometer flown from the U.S. and Peru aboard a U-2 aircraft. It is interpreted as due to the cosmological motion of the Milky Way Galaxy.

Measurements of the linear polarization of the CBR have been made at 9 mm and 30 mm. At 9 and 30 mm there is no polarization greater than 10^{-4}.

Measurements of the CBR spectrum were made in 1982 at White Mountain High Altitude Research Station in California. The measurements were made at five wavelengths (12, 6.3, 3, 0.9, and 0.3 cm), all below the peak of the spectrum. The radiometers used a single liquid-helium cold-load calibrator in order to reduce the systematic errors. The experiment is a collaboration of groups led by Giorgio Sironi

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(Milan, Italy) Reno Mandolesi (Bologna, Italy), R. Bruce Partridge, (Haverford College, Pennsylvania), and George Smoot (Lawrence Berkeley Laboratory). Many theories predict that a spectral distortion in the Cosmic Microwave Background is most readily observable in the Rayleigh-Jeans region. Measurements at White Mountain will continue, with an additional radiometer at 2-18 GHz.

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Title of Project: Double Beta Decay in ^{76}Ge

Person in Charge: F. Goulding

Scientific and Professional Staff: F. Goulding

Scope of Work; Goals and/or Major Results to Date

The purpose of this project is to develop and construct a germanium detector system having sufficiently low background to make possible observation of the decay of ^{76}Ge by the emission of two electrons with no accompanying neutrinos. The design is aimed to permit setting a minimum limit of 10^{24} years on the half life of the double beta decay of ^{76}Ge--a result that can be interpreted theoretically to correspond to a maximum mass for the Majorana neutrino of 1 eV.

^{76}Ge is a particularly convenient nuclide for the double beta decay experiment because it constitutes almost 8 percent of natural germanium and germanium detectors are the highest resolution radiation detectors available at the present time. Because LBL has played a major part in the development of germanium detector spectrometers and has unique capabilities for fabrication of special detector systems and the associated spectrometer electronics, a collaboration with a UC Santa Barbara group was a natural development.

Present experiments at other laboratories have established a limit of $> 10^{22}$ years for the decay half life of ^{76}Ge and an initial decision was made by the group to aim to raise this limit to $> 10^{24}$ years. A cluster of eight germanium detectors (four cryostats each containing two detectors) was chosen as a practical though difficult objective; it contains 7.5 kg of germanium and the double beta decay counting rate for a ^{76}Ge half life of 10^{24} years will be three counts/year. This last figure indicates the requirement for extremely low background and the design of the system has been focussed on extreme precautions to reduce background arising from natural radioactivities (U and Th series) and from cosmic ray-produced neutron-induced activities.

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Title of Project: PEP-4 Development and Operations Group

Person in Charge: A. R. Clark

Scientific and Professional Staff: A. R. Clark, S. C. Loken, R. Madaras, M. Pripstein, M. Ronan, T. Y. Fujita, J. Meneses, T. K. McGathen, J. A. Ortiz, L. W. Sherriffe, and I. W. Lee

Scope of Work; Goals and/or Major Results to Date

The TPC Operations Group to run and maintain the PEP-4 (TPC) experiment at SLAC has two components. One part consists of the ongoing electronic and mechanical maintenance, staffed by 6 engineers and technicians, plus costs of related supplies and expenses.

The Operations Group is also responsible for the maintenance and operation of the online computer systems and for supervision of the PEP-4 data reduction effort. The Physics Division personnel involved in these day-to-day operations are supported by the research program budget.

The Operations Group is also participating in the design, construction, and installation of a high-resolution vertex detector. The high resolution of this detector, along with reduced mass between the detector and the interaction point, will enhance the overall performance of the PEP-4 system by improving the momentum resolution through improved vertex resolution and by reducing confusion caused by photon conversions in the beam pipe and in the TPC pressure wall. Installation of the detector and modified beam pipe is planned for the summer of 1985.

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Title of Project: Large Detector Upgrades

Persons in Charge: (1) D. R. Nygren and P. J. Oddone; (2) G. Goldhaber and G. H. Trilling

Scientific and Professional Staff: (1) A. D. Bross, W. Hofmann, H. S. Kaye, R. J. Madaras, D. R. Nygren, P. J. Oddone, G. T. Przybylski, R. Sauerwein, and R. E. Avery; and (2) G. S. Abrams, R. W. Birge, P. Drell, G. Gidal, G. Goldhaber, J. Haggerty, D. A. Herrup, J. A. Kadyk, G. H. Trilling, D. E. Amidei, A. R. Baden, J. H. Boyer, F. E. Butler, M. S. Gold, L. J. Goulding, I. Juricic, P. C. Rowson, H. M. Schellman, W. B. Schmidke, P. D. Sheldon, and D. Wood

Scope of Work; Goals and/or Major Results to Date

1. Time Projection Chamber

The distortions observed in the PEP-4 TPC active volume have been studied intensively using the small laboratory TPC designed for this purpose. Additional studies of the G-10 fiberglass panels have been made using a high-volume electronically servoed electrostatic voltmeter. The hypothesis of low resistivity strands embedded within the bulk of the material has been confirmed. A corrective urethane coating has been applied to the fine field cage structures of the PEP-4 TPC.

During the current year work has been done to strengthen the mechanical support structure of the thin superconducting magnet and to clean and rebuild two of the six electromagnetic calorimeters which disintegrated during the last running cycle. A new gas will be used when the apparatus is again put into service.

2. The Mark II Detector Upgrade

The Mark II detector is being upgraded for its role as the first detector in the SLC, with turn-on expected in early calendar 1987. Major elements of the upgrade include a new central drift chamber, new endcap electromagnetic calorimeters, a new time-of-flight system and a new end door retraction system, all of which are to be available for checkout at PEP at the end of FY 1984 or the beginning of FY 1985. In addition, a new vertex detector and a small-angle luminosity monitor are to be constructed in time for installation at the SLC in late 1986.

Major LBL involvements in these efforts include full responsibility for the development and construction of the new endcap calorimeter (including both mechanical and electronic components), responsibility for the track reconstruction software for the new drift chamber, and collaboration with SLAC physicists on the development and construction of the vertex detector.

The endcap calorimeter is a major project involving the construction of two endcaps, each with 36 layers of alternating Pb sheets and 10,000 aluminium proportional tubes. Completion is expected in early 1985.

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Title of Project: Research and Development Using the TPC Concept

Persons in Charge: (1) P. Oddone; (2) P. Oddone; and (3) R. Enomoto

Scientific and Professional Staff: (1) P. Nemethy, P. Oddone, L. Stevenson, and T. Edberg; (2) P. Nemethy, P. Oddone, and W. Wenzel; and, (3) O. Chamberlain, R. Enomoto, R. Fuzesy, and T. Miki

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Berkeley, California

Scope of Work

Several new experiments become possible by using extensions of the TPC technique used in PEP-4. A few physicists from the PEP-4 group have an active R&D program to develop specialized time projection chambers to carry out these new measurements.

1. Tracking Imaging Cerenkov Counter

   An experiment to improve the muon neutrino mass limit, now equal to the electron mass, has been proposed by the group. It requires the development of a new kind of Cerenkov Counter, combining several technologies including a TPC, to make precise measurements of the pion and muon velocities in forward $\pi \to \mu\nu$. A letter of intent to do the experiment has been written to BNL since the optimum beam momentum for the experiment is about 2 GeV which is ideally suited for the AGS.

2. New Proton Decay Detector

   The group is attempting to develop ultra-high pressure TPCs as a way to obtain a dense and massive nucleon decay detector capable of identifying and measuring all possible nucleon decay products, except neutrinos. A high pressure TPC offers unique advantages as a nucleon decay experiment. At a pressure of 500 Atm. the density of Argon is 80 percent of the density of water, and the device becomes not only a tracking detector but also a detector capable of measuring total energies to the 1 percent level. Multiple measurements of dE/dx along the track (total energy) would completely identify the particles present in the decays. Such a detector could operate deep under the ocean in hydrostatic equilibrium or, most likely in the initial phase, deep underground in a pressurized cavern.

3. TOPAZ TPC Research and Development

   LBL is collaborating with the University of Tokyo on R&D and prototyping for the TPC to be used in the TOPAZ detector at TRISTAN, the Japanese electron-positron collider. LBL is active in the design and testing phases, but most of the construction will occur in Japan.

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Title of Project: Vertex Chamber Research and Development

Persons in Charge: (1) G. H. Trilling; (2) D. R. Nygren

Scientific and Professional Staff: (a) P. Drell, R. Fuzesy; and G. H. Trilling; and (2) R. J. Madaras, D. R. Nygren, and R. Sauerwein

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Scope of Work; Goals and/or Major Results to Date·

1. Mark II

LBL and SLAC scientists are collaborating in the development of a high resolution vertex drift chamber for use in the Mark II detector at SLC. This area was already pioneered with the present Mark II vertex detector and the goal is to provide a substantial improvement over the performance of that detector. The desired specifications are:

(a) $<$ 25 μm extrapolated impact parameter error
(b) $\leq$ 5 mr double track separation

At present this project is in an R&D phase and will be developed as a real full fleged component of the Mark II after an evaluation based on both the success achieved in the R&D and the status of alternative vertex detectors based on solid-state devices. The LBL part of the collaboration is particularly involved in the mechanical design initially of the test cells and eventually of the actual detector.

2. PEP-4 TPC

An evaluation of both current techniques and new or evolving ideas has been made to establish a direction for the development of a very high resolution vertex-tagging chamber. The studies have included scintillating glass fibers, micro-TPC's, and low drift velocity "jet" chambers. The latter seems to offer the best combination of properties but will require further laboratory work to confirm feasibility. If feasible, an extrapolated resolution of 25 microns at the vertex would be obtainable, about four times better than current drift chamber techniques.

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Title of Project: Room-Temperature Liquid Calorimeter Media

Person in Charge: M. Strovink

Scientific and Professional Staff: J. Carr and M. Strovink

Scope of Work; Goals and/or Major Results to Date

In searches of the chemical literature 2,2,4,4-tetramethyl pentane (TMP) has been identified as a possible room-temperature substitute for liquid Argon, the usual medium for charge collection in sampling calorimeters. Communications with a chemical firm have resulted in commercial production of the first pure samples of TMP outside a research laboratory environment.

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Construction of a sampling electromagnetic calorimeter module has begun for the purpose of testing TMP and other promising liquids in actual use for high energy physics measurements. If the early tests are successful, the group will proceed with the design and construction a multichannel sampling calorimeter system able to contain a high energy hadronic shower. Monte Carlo calculations indicate that the process by which uranium fission equalizes the hadronic and electromagnetic calorimeter responses is enhanced by the increased efficiency for neutron detection in TMP relative to liquid Argon. This effect will be studied experimentally to learn how to optimize the uranium content of a sampling TMP calorimeter.

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Title of Project: Neutrinoless Double Beta Decay of ^{100}Mo

Person in Charge: R. Kenney

Scientific and Professional Staff: M. Garnjost, R. Kenney, R. Muller, R. Tripp, B. Dougherty, J. Krivicich, M. Deady, and H. Nicholson

Scope of Work

A feasibility test on a neutrinoless double beta decay experiment using the nuclide ^{100}Mo is under way. The program in progress is the construction of a final prototype detector of approximately one tenth full size in order to acquire meaningful background data. This array will eventually become 10 percent of the full scale facility if no further design changes are required. The critical system parameters that must be within viable ranges are: 1) instrumental resolution, 2) electronic noise figure, and 3) background counting rate at the experimental site. Using a shield that was quite inadequate, they have reduced the measured background to a level that would yield a molybdenum lifetime of 10^{21} years measured with the full scale array. Several orders of magnitude improvement in background will be gained by siting the experiment underground and by completing the shielding in an adequate manner.

Development of stable high resistivity solid state detectors is under way and considerable progress has been made in solving problems and in establishing fabrication processes for making large diameter (~3 in.) thick (1.5 mm) silicon detectors of high purity (30 Kohm cm) without the aid of Li drifting. This technique is of great importance because it yields detectors that are stable in time, that have resolutions equal to Li drifted detectors, that have thin windows on both sides, and whose cost is 1/5 to 1/10 that of Li drifted detectors.

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Title of Project: Multipurpose Detector and Other Instrumentation R&D

Person in Charge: (1) V. Perez-Mendez; (2) A. Bross; (3) E. Lampo

Scientific and Professional Staff: (1) S. N. Kaplan, T. Mulera, V. Perez-Mendez, J. Morel, M. Razazan, and G. Schwartz; (2) A. Bross; and (3) E. Lampo and staff

Scope of Work; Goals and/or Major Results to Date

1. Multipurpose Detectors

Development work is being done on various types of radiation detectors. Emphasis is on gas-filled multi-electrode devices, but some work is also being done on new types of solid detectors. While the primary application of these detectors was in high energy and nuclear physics, they also found application in medical physics and in x-ray diffractometry.

Design studies of a drift collection calorimeter, in which the radiator and drift field shaping structure are combined in the form of lead glass tubing, were done using Monte Carlo shower simulation in cooperation with W. R. Nelson (SLAC). A highly resistive metallic layer is formed inside the tubing by surface reduction of the lead oxide in the glass in hydrogen atmosphere. This process, originally developed for medical work on positron emission tomography, results in a very uniform field shaping structure, allowing the efficient drifting of electrons to the detection wire chamber.

As part of the LBL-Pisa Collaboration in building a prototype detector, PISA is assembling the lead glass tube package and LBL is making the electronic readout system.

A program has been initiated to investigate the possible use of non-crystalline materials as solid state radiation detectors. Such detectors would not suffer from the size limitations imposed by the necessity of using single crystals of material as in conventional devices. Initial work was on the Vanadium Oxides. Other approaches that are being investigated are (a) semiconducting plastics, principally polyacetylene and (b) amorphous silicon.

2. Scintillating Glass R&D

Developmental work on cerium based scintillating glass is being pursued. Commercial glasses have been procured and their scintillation efficiency is being measured and will be used as a benchmark for LBL glass design work. The LBL glass fabrication program is starting by trying to duplicate the pioneering work of Anderson and Ginther. Owens-Illinois in Ohio is doing the actual glass fabrication; LBL hopes to make substantial improvements in the glass scintillation efficiency by using new ultra high purity fabrication techniques and materials. Glass suitable for drawing will be tested as the core glass for scintillating fiber waveguides.

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3. Physics Instrumentation

Continual design and development of advanced instruments, detectors and systems is necessary to meet the changing requirements of new experiments. Similiarly, there is constant evaluation of commercially available devices and instrumentation. As part of operating the equipment pool, inventory records are maintained of all equipment usage, new pool equipment is procured, and consultation is provided on any aspect of instrumentation. Ongoing maintenance, repair, and service are performed for all electronic instruments used in Physics Division Programs.

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Title of Project: Two-Beam Accelerator

Persons in Charge: A. Sessler and D. Prosnitz (LLNL)

Scientific and Professional Staff: D. Hopkins and J. Wurtele

Scope of Work

An investigation of a high-gradient two-beam accelerator (TBA) with the aim of determining whether it is an attractive possibility for the next generation of linear colliders has begun. Such an accelerator might be based on radiation generated by a free-electron laser (FEL). By operating at a frequency of about 30 GHz, one can probably attain gradients as high as 250 MeV/m and reduce the power requirements to 150 MW. As currently conceived, one of the TBA beams would be an intense, low-energy (about 3 MeV), long-pulse beam; the other--comprising the particles of interest--would consist of a few particles (about 10^{11}) in a short bunch, which is taken to very high energies (about 375 GeV) in about 1.5 km.

To explore the concept of TBA, they plan a balanced program of theoretical studies, table-top experiments with high-gradient structures, and further experimentation with the FEL at the Electron Laser Facility (ELF) at Livermore.

Goals and/or Major Results to Date

In support of the TBA concept, LBL has successfully operated the FEL at the ELF as a high-gain microwave amplifier. Using a 500-A electron beam from the Experimental Test Accelerator, they amplified a 40 kW input signal to 10 MW (at the fundamental 34.6-GHz frequency) in one run and to an estimated 100 MW in another. Significantly, the gain was achieved in the first 2 m of the 3-m wiggler, suggesting that higher gains are possible with a tapered wiggler.

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Title of Project: High-Field Superconducting Magnets

Person in Charge: C. Taylor

Scientific and Professional Staff: J. Zelver, W. Gilbert, H. Hassenzahl, J. Rechen, R. Scanlan, R. Althaus, S. Caspi, M. Helm, R. Meuser, K. Mirk, C. Peters, J. Royet, R. Schafer, and R. Wolgast

Scope of Work

In collaboration with Brookhaven National Laboratory (BNL), LBL is developing a magnet system for the Superconducting Super Collider (SSC) that is based on a 6.5 tesla 2-in-1 dipole fabricated with niobium-titanium superconductor operating at 4.5 K. [Higher fields (8-9 T) can be achieved with the same winding at 1.8 K or with a Nb_3Sn winding at 4.5 K.] LBL experimental models will be about 1 meter long, and BNL will build and test long models of LBL design, using LBL cable. In FY 1985, they will design and test 2-in-1 quadrupole models as well as dipole models. As part of this program, a collaborative effort with industry and academic researchers is aimed at producing superconducting cable with a higher critical current density than is now available.

LBL is also developing a self-energized local correction winding that can compensate for major field errors, particularly those due to persistent currents at low fields. In collaboration with an industrial firm, they are doing preliminary design and development of minimum-cost fabrication methods, as well as an independent cost estimate for complete SSC dipole magnets. LBL is prepared to provide essential R&D support to the SSC magnet program, regardless of which of several alternative designs is finally chosen.

Goals and/or Major Results to Date

Recent accomplishments have included the design of an SSC dipole magnet based on a 40-mm-bore-diameter winding and two layers of "wide" Nb-Ti cable, the testing of two 1-m-long models to verify details of the design, and progress towards the industrial manufacturer of high-J_c Nb-Ti. The preliminary LBL magnet design was the core of the most extensive of the three reference designs prepared for the SSC. The first model, D12-1, was successfully tested to 6.0 T in January 1984, and the second model, D12-2, was tested to 6.5 T in May.

In November 1983, LBL successfully tested the first high-field react-in-place Nb_3Sn dipole model, D10-A. This design used the first "internal-tin" Nb_3Sn cable made in the U.S.

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Title of Project: Beam Cooling

Person in Charge: G. Lambertson

Scientific and Professional Staff: D. Goldberg, W. Barry, W. Jackson, J. Johnson, B. Leskovar, C. Lo, F. Voelker, T. Henderson, H. Lane, and R. Weidenbach

Scope of Work

The technique of stochastic beam cooling involves detecting, for single particles, deviations from the mean position and velocity of the beam, then applying corrective impulses to the same particles at a position downstream. The development, production, and testing of components for stochastic cooling of antiprotons are being carried out in support of the Tevatron proton-antiproton collider project at Fermilab. In addition, LBL is pursuing improvements in this technology and its more general application to feedback systems for increasing beam stability in accelerators and colliders.

Goals and/or Major Results to Date

During the past year, LBL completed 2- to 4-GHz prototype arrays and tested both these units and the previously finished 1- to 2-GHz units with beam. Production is under way at Fermilab. Primary and secondary combiners for all arrays have been developed, and production of these units is proceeding at LBL. Input circuit designs are complete and assembly at LBL is scheduled. They have also begun to examine the design of feedback systems needed in the SSC to correct for the effects of noise and collective instabilities.

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Title of Project: Future Facilities Development

Person in Charge: J. Marx

Scientific and Professional Staff: J. Bisognano, M. Cornacchia, D. Douglas, A. Garren, B. Leemann, C. Leemann, and M. Zisman

Scope of Work

Considerable effort is being directed toward conceptual design aspects of the Superconducting Super Collider (SSC). To understand the link between the design of the 6.5-tesla dipole magnets being developed as part of the high-field superconducting magnets project and the design and performance characteristics of the collider, a thorough analysis of accelerator physics issues is required. LBL is studying these, not as separate topics of investigation, but as part of a comprehensive study of issues critically related to the architecture of a collider with defined performance goals. Important issues like the impact of magnetic multipole structure in the

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beam apertures and the impact of random magnetic imperfections strongly affect the overall performance of the collider. A close interaction between these studies and the magnet design effort has already led to improved designs and specifications.

The future facilities effort at LBL can be broadly divided into three parts relating to the SSC: basic design and parametric studies, accelerator physics and beam dynamics studies, and subsystems and component technology. Basic design studies involve analysis of machine parameters and their interrelationships with a view to understanding the tradeoffs among performance, technical risk, and cost. The accelerator physics studies concentrate on beam stability and involve critical analyses of performance-limiting phenomena, including expected field errors and collective effects. Subsystems under study will include the rf system, the power supplies, and the use of feedback systems.

Goals and/or Major Results to Date

Values for the basic parameters for the 6.5-tesla SSC magnet option have been proposed. These values meet the specifications for a luminosity of 10^{33} $cm^{-2}sec^{-1}$, with an acceptable number of collisions per crossing and an acceptable level of synchrotron radiation. These parameter values were adopted for the SSC Reference Designs. LBL accelerator physicists formed the core of the SSC Accelerator Physics Group and, as such, contributed significantly to the Reference Designs effort. Investigations on long-term beam stability will require improved methods for tracking studies, which will be developed as part of this project.

During the first half of 1984, LBL served as host institution for the SSC Reference Designs Study, providing support of sufficient quality and depth to allow the study to complete its substantial effort on schedule. The task groups responsible for cost estimates and report production were headed and staffed by LBL personnel.

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Award No.: DE-AC03-76SF00515

Title of Project: Experimental Group A

Person in Charge: C. Prescott

Scientific and Professional Staff: W. Atwood, E. Bloom, N. Boguslaw, B. Brucaud, R. Clare, S. Cooper, A. Courau, H. DeStaebler, R. Dubois, E. Elsen, G. Godfey, A. Ogawa, R. Pitthan, L. Rochester, O. Saxton, A. Schwarz, D. Sherden, K. Wacker, and C. Young

Scope of Work

Experimental Group A pursues two large experimental programs; the first involves experiments at PEP utilizing the DELCO apparatus; and the second experiments at DORIS utilizing the Crystal Ball.

The group presently conducts experimentation at PEP with the DELCO detector and experimentation will continue into FY 1986. In the later years the majority of effort will be directed at data analysis. Members of the group are also active in preparations for future projects at the SLC. The main effort beginning in FY 1984 was the design, prototyping, and testing of drift chambers for the new SLC detector (called "SLD"). This design effort has begun, and the drift chambers will enter the construction phase in FY 1986. Some members of the group will continue to contribute to alignment problems for the beam transport of the SLC.

Representing a major experimental program in e^+e^- physics, the Crystal Ball is a non-magnetic detector designed to measure photon and electron (positron) energies and directions with high precision. It also measures the angles of charged particles. The group contributes to a large collaboration of physicists consisting of 12 institutions. Though the detector was mainly built by the SLAC Crystal Ball group, Stanford-HEPL, and CIT group, the entire collaboration cooperatively runs it and cooperatively analyzes the data.

Goals and/or Major Results to Date

The main effort in FY 1983 was the operation of DELCO at PEP and the analysis of data obtained from that experiment. The online data acquisition system was streamlined, thereby significantly increasing the amount of data. The initial preparations for a tracking chamber for the SLD began in late FY 1983.

Group A will continue to operate DELCO at PEP and analyze data. Operation of DELCO will continue until FY 1985, and the analysis of the data will continue beyond FY 1985. The major efforts of the group will transfer to the SLD and Mark II projects at SLC.

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The Crystal Ball has been primarily involved in taking data at DESY, analysis of DORIS and SPEAR data at SLAC, and improvements to the detector. Data analysis has been heavily concentrated at SLAC. During thé last year major improvements were made to the experiment. These improvements are expected to significantly expand the physics output of the experiment at DESY.

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Title of Project: Experimental Group B

Person in Charge: D. Leith

Scientific and Professional Staff: V. Ashford, P. Ashton, S. Csorna, W. Dunwoodie, M. Grairna, P. Kunz, A. Miyamoto, G. Oxoby, B. Ratcliff, L. Shapiro, L. Shimomura, G. Tarnopolsky, A. Waite, and S. Williams

Scope of Work

The research interests of Experimental Group B are studying the spectroscopy of light quarks in a systematic way and obtaining some insight into the forces involved in the strong scattering process. Such experiments demand a non-restrictive, unbiased selection of the final states produced in hadronic collisions, a requirement well matched to the properties of the LASS spectrometer, and sophisticated analysis machinery to extract the scattering amplitudes from the measured cross sections--machinery developed by this group over the past decade.

The group is also interested in the potential physics opportunities at the SLC. This new machine will present not only the well publicized, very exciting program to study the weak interaction, but will also allow detailed studies of the strong interaction and of quark hadronization processes that have been up to now impossible.

Goals and/or Major Results to Date

The main group activity centered on preparing the analysis codes and finalizing the calibration and alignment constants prior to processing some 250,000,000 events from LASS experiment E-135. The optimizing of the production codes for E-135 data and the final tuning of the constants are expected to be completed in FY 1984.

The sub-experiment on $\bar{K}^0\pi^+\pi^-$ final states in E-132 was completed and several new strange quark states were observed.

The preliminary design of a new microprocessor called the 3081/E was settled, and a CERN/SLAC collaboration was set-up to complete the design, build the first prototype, and fabricate the devices.

The group took a large role in the SLC workshop, and was a major participant in the group pushing for a new detector for SLC--the SLD.

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Several members of the group were deeply involved in assignments on the SLC and will continue to be well into FY 1986.

Good progress was achieved in the detector R&D program.

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Title of Project: Experimental Group C

Person in Charge: R. Larsen

Scientific and Professional Staff: G. Bartha, D. Briggs, A. Boyarski, M. Breidenbach, F. Bulos, T. Himel, R. Hollebeek, M. Jonker, A. Lankford, N. Lockyer, V. Luth, S. Weisz, R. Wilson, and J. Yelton

Scope of Work

Research Group C is engaged in experimental studies of electron-positron colliding beam phenomena, the development of new particle detection devices and techniques, and accelerator design and development.

Goals and/or Major Results to Date

The Mark II collected 120 inverse picobarns at PEP at an energy of 29 GeV center-of-mass energy. It is expected that an additional 60 to 80 inverse picobarns will be collected at PEP at the same energy. Analysis of this data and of SPEAR data has resulted in new and improved contributions to the field of elementary particle physics.

In addition to the many physics results, design of all major components of the upgraded Mark II has been completed and fabrication commenced.

A new drift chamber, one new end-cap detector, and a new time-of-flight system will be completed. The Mark II will move off the PEP beam line in the spring of 1984 for further improvements. This work is a continuation of the upgrade of the Mark II for the PEP and SLC experimental programs.

The installation and testing of the upgraded detector components for the Mark II will continue until the Mark II moves back to the PEP beam line in the winter of 1984-85. The upgraded detector will begin collecting useful data at PEP towards the end of this cycle.

These improvements will aid in the study of heavy quark production and decay. PEP-21 will also execute the proposal to search for supersymmetric particles.

In spring 1986 the Mark II will be removed from the PEP beam line to commence the move to the SLC experimental area.

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Title of Project: Experimental Group D

Person in Charge: R. Mozley

Scientific and Professional Staff: K. Bunnel, R. Casell, D. Coward, S. Dado, N. Hermes, A. Odian, and W. Toki

Scope of Work

This group is presently engaged in experiments using the Mark III detector at SPEAR.

The program envisions a study of charmed quark states including charmonium decays, D-meson decays, a search for the F-meson, and charmed baryon states and decays. A study of tau decays is also contemplated.

Goals and/or Major Results to Date

Many physics results were obtained during FY 1983, including but not limited to the collection of a combined total of 2.7 million decays recorded, spin parity analysis in progress, the observance of a new resonance in one of the channels, and the analysis of these and other channels in progress.

Approval was given by the SLAC Management for a minibeta installation at SPEAR which will improve luminosity by a factor of 3. The summer of 1984 will be devoted to the installation of minibeta.

A project is also under way to design (not build) an improved inner chamber for the Mark III detector.

The fall of FY 1984 run will be primarily devoted to resuming operation with the minibeta. After normal operation is acheived, work will be done in obtaining more data.

If the minibeta improves the luminosity appreciably, there may be a move to make an even more detailed study of psi decays, approximately 20 million events, since this number would be required to make a definitive search for glue balls in the radiative decays.

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Title of Project: Experimental Group E

Person in Charge: M. Perl

Scientific and Professional Staff: T. Barklow, D. Burke, J. Dorfan, G. Feldman, G. Hanson, K. Hayes, W. Innes, C. Matteuzzi, and J. Witthaus

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Scope of Work

Group E pursues four fields of research. One field consists of the study of the physics of electron-positron annihilation at high energy; with emphasis on the properties of particles containing the heavy quarks and on the search for new particles.

The second field of research concerns the fundamental nature of the charged leptons (the electron, muon, and tau); and the search for heavier charged and neutral members of that lepton family.

The third field of research concerns the development of new types of particle detectors which allow more precise measurements of the properties of the new leptons and hadrons and also allow more extensive searches for new particles.

The fourth field is the search in macroscopic matter for fractional electric charges--such charges could come from free quarks or from fractionally charged leptons.

Goals and/or Major Results to Date

One of the group's major efforts was extensive studies of e^+e^- annihilation physics using the Mark II detector at PEP. One result from this large data sample was the measurement of the lifetime of the B mesons, which is the simplest meson containing the heaviest known quark, the b quark.

The other major effort of the group is the upgrading of the Mark II detector for use at the Stanford Linear Collider. The group is carrying the major responsibility for the construction of the new drift chamber and is participating in many other areas of the upgrade program.

Development work on high spatial resolution drift chambers continues. The goal is the construction of an ultrahigh spatial resolution chamber for use at the SLC.

A new experiment, the ASP single photon experiment, was developed and accepted for PEP which consists of looking for events containing a single photon and two neutrinos or two neutrino-like particles.

The fractional charge apparatus work continues. The experiment will continue through the FY 1985 - FY 1986 time frame.

In the FY 1985 and FY 1986 time frame, the data analysis of Mark II at PEP should be complete. A program for upgrading the Mark II for SLC will continue and approach completion.

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Title of Project: Experimental Group F

Person in Charge: D. Ritson

Scientific and Professional Staff: G. Chadwick, S. Clearwater, K. Lau, H. Lynch, and F. Muller

Scope of Work

Experimental Group F is the SLAC research physics group collaborating on the MAC detector at PEP with a primary responsibility for off-line data management and analysis.

The group is concerned with the development of new hardware for improving this large device and with the extraction of the physics from the data accumulated at PEP.

Goals and/or Major Results to Date

The group concentrated on the running and analysis of results of the MAC detector at PEP. Substantial luminosity was accumulated and a wide range of publications resulted including fragmentation studies, radiative leptonic processes, a preliminary measurement of the B-lifetime, a SUSY search, and a high statistics muon asymmetry measurement. Additionally an investigation was made of helium-filled proportional chambers as a device for investigating monopoles in the Cosmic Radiation.

The group expects to build and install in the MAC detector a pressurized vertex chamber that will be sensitive as close as 3.5 cm to the beam-line. This should allow for the studies of the B lifetime and other lifetime measurements with a precision substantially improved over any previous work. The design will, with some hardware modifications, permit an improved continuation of the present SUSY search and provide enhanced precision from further running.

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Title of Project: Experimental Group G

Person in Charge: S. Wojcicki

Scientific and Professional Staff: G. Irwin, D. Porat, and J. Ritchie

Scope of Work

The major effort of Group G at SLAC is concerned with data taking and data analysis using the DELCO detector at PEP. The experiment is a collaboration with SLAC Group A and another group from the California Institute of Technology and emphasizes the detection of direct electrons by means of a large solid angle Cerenkov counter. The detector can also do pi-K separation above 2.5 GeV when the Cerenkov counter is filled with isobutane. The main physics goals of the program are study of heavy quark production, search for new phenomena, study of jets, investigation of leading particle correlations, and study of 2-photon interactions.

Goals and/or Major Results to Date

There have been some improvements in the on-line software system which enables one to locate the hardware malfunctions much more rapidly. In addition, some minor changes were made in the inner drift chamber system in order to reduce the frequency of Geiger pulses and spurious hits. A laser fiber optics system for calibration of the time-of-flight counters was completed and calibrated.

All of the running time during FY 1984 has been with the nitrogen filling of the Cernekov counter. This lighter gas permits exploration of the whole electron spectrum from the charm and bottom decays at a slight sacrifice of the pi-K separation. A paper on the direct electron production has been submitted for publication to the Physical Review Letters.

Data taking may continue during the FY 1985 - FY 1986 period. It is anticipated that the completion of analysis will take one to two years after the end of the data taking.

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Title of Project: Experimental Group Bubble Chamber/SLAC Hybrid Facility Operations

Person in Charge: J. Ballam

Scientific and Professional Staff: M. R. Armenteros, J. Bartelt, K. Braune, D. Cords, P. Ferrell, R. C. Field, T. Glanzman, and K. Moffeit

Scope of Work

The group performs basic physics research using the SLAC Hybrid Facility (SHF). The 40" Hydrogen Bubble Chamber and electronic detectors comprise the apparatus of the facility. In addition to the group's own research program, it provides assistance to non-SLAC users in the design and carrying out of physics experiments. The group has developed and operates supplemental detector systems as a facility for collaborators and users.

The group is now a member of the collaboration to upgrade the Mark II for the SLAC Linear Collider. The group is developing detector systems for the Mark II upgrade.

Goals and/or Major Results to Date

Data taking commenced for BC 75, and the film taken was scanned and measured. It is expected that all scanning and measuring will be completed in the FY 1984 time frame.

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The high resolution camera has been worked on to improve the optical quality.

A final paper on the analysis of charmed-particle events in BC 72/73 was prepared with the group's collaborators and submitted for publication.

Analysis of strange particle inclusive production was completed and a paper was submitted for publication.

Work on the design of a large liquid Argon bubble chamber to detect proton decay was done in collaboration with the cryogenics group.

The group joined the Mark II at SLC collaboration and began work on this project. In addition, technical assistance was provided for the SLC.

It is anticipated that in the FY 1984 - FY 1985 time frame, all of the analysis of the BC 72/73/75 experiments data will be completed. Several publications are expected from these results. It is also projected that work will continue on the improved Mark II detector; and technical assistance to the SLC will continue to be provided.

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Title of Project: Theoretical Physics Group

Person in Charge: S. Drell

Scientific and Professional Staff: I. Antoniadis, H. Aoyana, T. Banks, R. Blankenbecler, D. Boyanovsky, S. Brodsky, J. Bugger, F. Gilman, W. Goldstein, J. Hagelin, D. Horn, C. Ji, H. P. Noyes, C. Ong, H. Quinn, M. Peskin, N. Sawicki, M. Soldate, Y. Tsai, and M. Weinstein

Scope of Work

The theoretical research program is in part directly related to SLAC's experimental program and in part strives to develop new concepts and formal techniques.

The research program of the theory group pursues a number of topics, spanning the field of particle physics from quantum gravity to better limits on the tau neutrino mass from analysis of hadronic decays of the tau.

Broadly grouped, the studies in progress or planned on the structure of field theory include the analysis of quantum gravity in 2- and 3-dimensions from the viewpoint of the Schrodinger wavefunction and its relation to the theory of strings; the search for new ways to generate masses of quarks and leptons; and a continuing program on the structure of theories, leading dynamically to the formation of a space-time phase.

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Goals and/or Major Results to Date

New algorithms for computer simulations and for variational and analytic techniques for solving field theories, including lattice gauge models, and calculating such properties as mass spectra, phase points, and properties of quantum electric devices are being developed and applied.

General and phenomenological studies of strong processes, new forces, and particle structure on the mass scale above 1 TeV are in progress with a number of different approaches as applicable to Z^0 decay branching ratios and to interactions observable at the proposed super collider.

There is an extensive ongoing program of QCD studies of the bound state problem, including the "intrinsic" heavy quark contributions and contributions from supersymmetric particles and "hidden color" degrees of freedom in nuclei.

A review of higher radiative corrections as deduced from renormalization group studies and an extension of "zero range" covariant scattering theory are also in progress.

The Theoretical Physics group expects to continue to pursue these avenues of research well into the FY 1985 - FY 1986 time frame.

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Title of Project: SLAC Computing Services/Computation Research

Person in Charge: R. Taylor

Scientific and Professional Staff: R. Beach, A. J. Cook, M. Fisherkeller, J. Friedman, D. Gustavson, and J. Steffani

Scope of Work

The effort of this project is divided into two major areas: (1) research and development on computer application techniques for physics, and (2) computer operations.

1. Computer Applications:

   The work of the Computation Research Group can be roughly divided into two broad categories: (a) basic research in computer science and statistics, and (b) innovative computer applications.

   Current research falls into seven broad categories: (a) statistical and computational techniques for data analysis, (b) programming language development, (c) microcomputer and microprocessor techniques, (d) numerical mathematics, (e) interactive graphics, (f) computer aided design, and (g) hardware and software standardization.

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The goal of the innovative computer application is computer programs or computing systems that solve specific and immediate problems and are directly available for physics applications.

2. Computer Operations:

The computer operations effort is concerned with the operation, maintenance, and development of the SLAC Central Computing Facility, which consists of VM service on an IMB 3081-K computer system. Effort on this system includes: Scheduling, dispatching, operating, and maintaining the system such that VM services are provided to the user 165 hours per week; planning for and coordinating the installation of additional hardware and software systems as needed; and providing assistance to the user.

Goals and/or Major Results to Date

Computer applications work in FY 1983 has included implementation of two major projects: The SLAC Unified Graphics System and MORTRAN (Programming Language development, applications). In addition, there has been considerable work in a number of other areas including: microcomputer techniques, program improvement and maintenance, local area networking, text processing, FASTBUS, and beam optics. Computer operations work during FY 1983 included improving and extending the VM/370 system, as well as the implementation of a number of other projects. In the future, work will continue on the major projects of the group, including FASTBUS, integrating the range of small computers with the central facility, networking activities, and continued enhancement of central VM services.

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Title of Project: Data Analysis Group

Person in Charge: J. Brown

Scientific and Professional Staff: G. Bower, M. Huffer, A. Leino, and P. Malley

Scope of Work

The objectives of the Data Analysis Group are twofold. The first is to design, construct, operate, and maintain scanning and measuring equipment for the analysis of film recorded data from bubble chamber experiments. This also includes not only manually operated, but also partially automated devices, and such work as hardware and software modifications to film measuring machines to permit precise profile measurements of laminations to be used in constructing SLC arc magnets. The second function is to acquire and support hardware and software for various computer systems. Currently this includes 22 VAX computer systems at PEP and elsewhere, as well as several hundred computer terminals.

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Goals and/or Major Results to Date

During FY 1983 automatic track following was added to a fourth measuring machine. The scan table software was modified to permit examination of two high resolution views from the 40" bubble chamber as part of the BC-75 data reduction effort.

In addition, production scanning and measuring for BC-72/73, a bubble chamber experiment measuring charmed particle photoproduction and lifetimes using high resolution optics, were completed. Additional VAX computer systems are expected to be utilized in connection with SLC, either as instrumentation and control machines for the collider itself, or as data acquisition systems for experiments. Work will continue on providing a full-function integrated local area network connecting the VAX computers to the central IMB facility.

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Title of Project: Accelerator Operations Department

Persons in Charge: B. Richter and J. Paterson

Scientific and Professional Staff: R. G. Gilbert, J. Harris, J. Jasberg, T. Martin, G. Nelson, J. Paterson, R. Stege, L. Stein, J. Taylor, and D. Tsang

Scope of Work

The Accelerator Operations Department includes Linac, PEP, and SPEAR operations. These programs are described below:

1. Linac Operations: Included in this subactivity is the effort expended to operate and maintain the two-mile accelerator and the Beam Switchyard complex. Both the accelerator and the switchyard continue to operate very reliably and the maximum beam energy continues to edge upward as relatively low power klystrons (20 and 30 MW) fail and are replaced by higher power (38 MW) tubes and the accelerator is operated in the SLED I mode.

2. PEP Operations: Since PEP has become operational, development has been directed toward improvements to PEP as well as to more general problems of colliding beam and storage ring systems. Much of this latter effort focus is associated with the SLC. PEP-associated R&D effort is, in general, going into improvements in reliability, operational convenience and efficiency, reducing operating costs, and optimizing performance and effective luminosity.

3. SPEAR Operations: The SPEAR group is responsible for the operation, maintenance, and improvement of the electron-positron colliding beam facility, SPEAR. The group works with the Stanford Synchrotron Radiation Laboratory in the development of SPEAR as a source of synchrotron radiation.

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Goals and/or Major Results to Date

The Linac was operated a total of 769 shifts in FY 1983 with 272 shifts of this total run at 180 pps, 28 shifts at 120 pps, and the balance of 469 shifts at 60 pps. Operating with this mix of repetition rates yielded approximately 27 percent of the maximum feasible number of electron pulses deliverable during the twelve month period. At PEP, during FY 1983, 80 percent of the available time was devoted to physics run with the remaining 20 percent used for accelerator development and maintenance. Operations at SPEAR were divided 50:50 between the high energy physics program and the provision of synchrotron radiation for the Stanford Synchrotron Radiation Laboratory.

The FY 1985 schedule calls for operating the Linac a total of 560 shifts, 70 of which will be run at 180 pps and 490 shifts at 60 pps. At PEP during FY 1985 and FY 1986 it is expected that results from the R&D program as well as minor modifications effected under general modifications will gradually improve reliability, efficiency, and luminosity. It is anticipated that SPEAR operations will continue to be divided 50:50 between SP-32 and SSRL.

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Title of Project: Accelerator Research & Development

Person in Charge: B. Richter

Scientific and Professional Staff: M. Allen, K. Bane, J. Campisi, R. Erickson, Z. Farkas, H. Hanerfeld, W. Herrmannsfeldt, R. Noble, P. Wilson, and S. Yu

Scope of Work

Included in this subactivity are three continuing research projects, the objectives of which are near-term improvement programs leading to higher beam energies, intensities, and reliability. Another part of this program is the development of higher power klystrons for use on the SLC.

1. Klystron Tube Development: This program deals with improvements in the reliability, efficiency, output power, and pulse length of various kylstrons built at SLAC. These efforts will result in savings in power and tube replacement costs.

2. Studies in Accelerator Physics: The Accelerator Physics Department carries out research and development work in a number of areas, including the following: Electron-optics calculations for SLAC gun designs for accelerators, klystrons, and novel power sources for future colliders; design of high current guns using cesiated gallium arsenide cathodes working by photoemission from laser light; optics design of collider arcs and final focus systems; and accelerator physics problems related to the conceptual design of the SSC (Superconducting Super Collider).

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3. High Power Beam Intercept Studies and Instrumentation: This program is conducted to develop the peripheral devices necessary for the instrumentation and control of the electron beam. Studies of monitoring and control devices are continued under this program.

Goals and/or Major Results to Date

The 50MW klystron design was selected as the primary one for SLC application. Accordingly, a dozen such tubes were built during FY 1983. Development work on the 50 MW klystron is continuing during FY 1984.

In accelerator physics, progress was made in all areas of investigation including the development of improved configurations and increased luminosity for PEP; and improvement in positron generation for PEP and SPEAR.

In FY 1985-86, once a final choice has been made on which klystron will be used in the SLC, that tube will go into full production. The SSC accelerator physics problems studied during FY 1984 will continue. An improvement program on the main linac injector will be studied with a view to easier operation under SLC requirements.

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Title of Project: Experimental Facilities Support

Person in Charge: R. Taylor

Scientific and Professional Staff: R. Blumberg, D. Fryberger, R. Gearhart, F. Halbo, E. Johnson, L. Keller, J. Murray, J. Va'vra, and H. Weidner

Scope of Work

Experimental Facilities Support includes the effort of the Experimental Facilities Department (EFD), the Electronics Department, and provision of utilities for the research area.

Experimental Facilities Department: EFD is responsible for the engineering support, installation support, and operation and maintenance of certain facilities in the fixed-target area and the SPEAR and PEP interaction areas. Facilities in the fixed-target area presently include the backscattered laser beam to the Hybrid Bubble Chamber, the End Station A spectrometers, and three test beams.

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Electronics Department: The principal purpose of the Electronics Department is to provide SLAC-wide support in the areas of electronics shop services, accelerator machine maintenance, instrument loan and repair, and Research Area support. The Electronics Department currently consists of the following major groups: Accelerator Electronics Department (AEE), Accelerator Electronic Maintenance (AEM), Electronics Instrumentation Engineering (EIN), Laboratory Electronics Pool (LEP), Electronic Production and Coordination (EPC), and Research Division Support (RDS).

Utilities and Utility Engineering for Research Area: The research areas require large amounts of electrical power and cooling water to operate the secondary beam lines and the large experimental detectors. These utilities and their associated systems are provided and maintained as a service to the experimental user.

Goals and/or Major Results to Date

During FY 1983, the work of the Experimental Facilities Department staff included consultation, proposal analysis, design, setup, operation, and equipment removal. Work with facilities during this period included the HRS at PEP, the SLAC Hybrid Facility (SHF), the Mark III Magnetic Detector for SPEAR, and the test beam facilities. Experiment BC 75 was nearly completed in the backscattered photon beam. A new hydrogen target was constructed and installed in End Station A for E-136.

In FY 1985 detailed design of the experimental set-ups in the SLC IR will be in process, as will planning for their installation. At PEP, the Mark II detector will begin taking data in the new configuration which will also be suitable for SLC. There will be considerable work on the SLD as well as various other projects.

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Title of Project: Cryogenic Operations

Person in Charge: R. Watt

Scientific and Professional Staff: P. Cutler, R. Davis, H. Petersen, R. Rinta, and D. Tolaska

Scope of Work

The Cryogenic Operations Group has the responsibility for the operation, maintenance, and improvement of the Central Helium Facility and the cryogenic systems of the Mark II (PEP-5), HRS (PEP-12), and TPC (PEP-4).

These responsibilities include the areas of mechanical, electromechanical, electronics, and computer control with the group providing most of the necessary design, development, and fabrication.

The Central Helium Facility is the source of purified helium gas used at the large superconducting detectors at PEP. The engineering staff of the group is providing preliminary consultation on both cryogenic and superconducting systems planned for SLC and SLD. Group engineers and technicians are involved in developing and fabricating gas support systems for various Group B projects which support the SLD project.

Also, the Cryogenic Operations Group staff consults and provides design, fabrication, and testing for other high energy physics laboratories when required and approved.

Goals and/or Major Results to Date

The Central Helium Facility operated at full capacity in FY 1983. Improvements have been made including the installation of a larger helium compressor which has increased facility capacity. The facility will continue to operate HRS and TPC through FY 1986. It will continue to be upgraded as needed and may be used in superconducting testing (SLC, SLD) as necessary.

The Cryogenic Operations Group will participate in planning the move of Mark II into SLC and during FY 1986, will be very much involved in the actual moving and installation of Mark II at SLC.

The SLC and SLD are expected to have large cryogenic systems as part of their operating systems. It is anticipated that in FY 1985 and 1986 considerable effort will be required from the Group's engineering and technical staffs in getting these projects in operation.

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Title of Project: MAC Operating Group

Person in Charge: R. Taylor

Scientific and Professional Staff: R. Coombes, R. Messner, and D. Wiser

Scope of Work

The MAC operating group was formed in January 1981 for the purpose of establishing and maintaining the MAC detector as a viable and efficient piece of apparatus for performing experiments at PEP.

This unique detector, which has been designed for calorimetry and lepton identification, is currently accumulating useful physics data.

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The activities of the group fall into three categories:

1. Maintaining and calibrating the existing detector,
2. Completing systems that are not yet fully operational,
3. Increasing the power of the device in terms of its physics capabilities by developing new systems and upgrading existing ones.

In all of these activities, the operating group works in close association with collaborating physicists and their technical staffs.

Goals and/or Major Results to Date

During FY 1983 the emphasis of the group was two fold: first, the efficient operation of the detector for data gathering, and second, improvements to the detector which point to specific physics goals. The ongoing analysis of the data sample was used to pinpoint areas in the apparatus which could be improved for reliability and quality of the data recorded. The Operations Group also took the primary responsibility for the design, construction, and installation of a new small angle tagging device for the detector.

The main effort will continue to be the efficient operation of the detector and the installation of new systems to increase its effectiveness. Work is currently in progress to develop a high resolution vertex chamber and electronics which will be installed inside the existing central drift chamber. The system is meant to improve MAC's current measurement of the B lifetime.

Long term R&D work will continue to study possible upgrades to the endcap calorimetry and the use of photodiode readout for BGO crystals which might replace photomultiplier tubes in calorimetric devices.

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Title of Project: Applied Physics - Physical Electronics

Person in Charge: R. Taylor

Scientific and Professional Staff: E. Garwin, E. Hoyt, F. King, R. Kirkby, A. Nyaiesh, A. Roder, and C. Sinclair

Scope of Work

The Physical Electronics Group (PEL) has a long history of applying sensitive and sophisticated techniques of ultrahigh vacuum, surface physics, electron physics, and solid state physics to problems of crucial importance to SLAC. PEL is concerned with development of novel sources for the accelerator, development of the high peak current gun for single pass collider use, detection and monitoring devices useful in particle physics, and a wide spectrum of surface physics techniques. In addition, PEL fulfills various service functions for the Laboratory in the areas of vacuum coating, optical absorption and reflection measurements, materials research, metallurgical analyses, and various special technique areas. PEL is heavily committed to research on increased polarization of spin-polarized photo emission sources, surface physics studies of niobium as applied to rf superconductivity, and study of low secondary emission coatings applied to klystron windows.

Goals and/or Major Results to Date

Since FY 1981, the surface physics and metallurgy facitiies have been increasingly applied to problems of klystron production, and in FY 1983 a program to evaluate solid state cathodes a selectron sources for rf power generation was begun.

The research and development of the SLC high current polarized electron gun and its associated laser is in progress. The program to grow the chalcopyrite $CdSiAs_2$, widely believed to be the best candidate photo emitter for highly polarized beams has been successful, with the first identifiable layers of this compound being synthesized near the end of FY 1983.

The SLC polarized gun and laser will be completed and delivered to the injector area for actual operation in FY 1986.

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Title of Project: Applied Physics - Low Temperature Materials Research (LTMR)

Person in Charge: R. Taylor

Scientific and Professional Staff: S. St. Lorant

Scope of Work

The LTMR Group is concerned with the application of low temperature physics to the high energy physics program. This includes evaluation of materials, the design, construction, and testing of various devices, as well as the study of the solid state at low temperatures insofar as this relates to high energy physics. The group manages all large scale helium procurements and distribution and furnishes liquid and gaseous helium to qualified users. An increasingly important part of the activities is the provision of engineering and technical support for various projects where the special expertise of the group is best applied.

Goals and/or Major Results to Date

Current emphasis of the group includes the rf superconductivity research with various cavity geometrics and materials and the final focus quadrupoles for SLC and related work. For the quadrupoles, a study of the intersecting ellipse type of geometry showed an inherent sensitivity of the design to wire placement accuracy. Various winding methods, tooling and epoxy formulations were tried in order to determine the parameters which determine the precision achievable. The tests showed clearly that this type of winding geometry results in unacceptably large errors in the field quality of a quadrupole, and a recommendation was made to abandon this particular arrangement.

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Title of Project: Applied Physics - Radiation Physics Research

Person in Charge: R. Taylor

Scientific and Professional Staff: K. Barta, T. Jenkins, R. McCall, W. Nelson, R. Shore, and W. Swanson

Scope of Work

Radiation Physics Research is that part of the general SLAC health physics program which is devoted to the study of new methods and devices for radiation dosimetry, analytical techniques that can be used to predict radiation levels, and pure physics experiments designed to give results useful in the health physics field.

Goals and/or Major Results to Date

Research results on muon shielding at high energies were published in a paper in 1983. Gas bremsstrahlung studies were done in collaboration with LBL and KEK which indicated that this is not a source of concern for most electron accelerators.

Other studies in progress include SLC-related radiation problems, self-shielding of the SLD detector, multiple scattering of fixed-target geometrics, design of the scintillation survey meter and the ionization chamber survey meter.

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Title of Project: Applied Physics - Magnetic Optics

Person in Charge: R. Taylor

Scientific and Professional Staff: K. Brown

Scope of Work

The Magnetic Optics Group provides analysis and develops and maintains computer programs related to the beam optics of charged particle accelerators and their associated beam transport systems.

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Goals and/or Major Results to Date

Ongoing studies conducted by the group are related to the understanding of nonlinear properties of beam transport systems so as to design ways to compensate or correct for these effects in storage rings, colliding linacs, and other machines.

The current emphasis of the group has been directed towards the design of magnetic optical systems for the SLAC Linear Collider.

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Title of Project: Miscellaneous Research Support

Person in Charge: R. Taylor

Scientific and Professional Staff: None permanent

Scope of Work

This category of effort consists of several small but important programs of the labortory. These include: 1) Hazardous Equipment Committee, 2) Experimental Program Advisory Committee, 3) Users' Support, and 4) Film Processing.

The Hazardous Equipment Committee is composed of SLAC physicists and engineers. This Committee is responsible for the design review of all potentially hazardous apparatus intended for use at SLAC and for advising the SLAC Director on the results of their findings.

The Experimental Program Advisory Committee, at present, consists of physicists from SLAC and other institutions. This Committee meets periodically to review experimental proposals received at SLAC and to advise the SLAC Director on the scientific merit of the proposals.

The Users' Support effort is composed of a small and varying group at SLAC personnel whose function it is to provide administrative assistance to outside users of SLAC facilities. Included in the services provided are secretarial services and assistance with proposal preparation. Provision for standard magnets, beam defining elements, targets, etc., is included in the Experimental Facilities Operations budget and is provided to users at no cost.

The film processing activity was initiated in early 1971 with surplus equipment obtained from PPA and LBL. Experimental photographic film, which is exposed in the SLAC Hybrid Bubble Chamber is processed by this small group. This effort requires about two personyears each year.

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Goals and/or Major Results to Date

As SLAC completed its sixteenth full year (FY 1983) of experimental research operations, the degree of outside user participation in the program continued at a high level. The cumulative record indicates that a total of eighty-six outside institutions (fifty-seven U.S. and twenty-nine foreign) have participated in the SLAC experimental program.

The distriubtion of experiments between outside users and inhouse SLAC groups during FY 1983 was similar to the general pattern that has characterized the SLAC program in the recent past. In FY 1983, roughly 70 percent of the beam hours in electronics experiments were utilized by outside users.

The Users' Support Group expects to continue to be responsive to the administrative needs and designs of SLAC users and prospective users. It is anticipated that the past pattern of outside use will continue.

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Title of Project: SLC Research and Development

Person in Charge: J. Rees

Scientific and Professional Staff: R. Bell, G. Bowden, C. Cook, W. Davies-White, G. Fischer, A. Hutton, R. K. Jobe, A. Keicher, W. Oren, J. Sirois, R. Steining, and J. Walling

Scope of Work

The SLC Research & Development group carries out experimental and theoretical studies on the SLC technique of particle acceleration, i.e., research and development in support of construction and operation of the SLC. The group is currently concentrating its efforts in the following areas: the conceptual design of linear colliding beam systems; an experimental program to study the effects of the SLAC linac on the emittance of single bunches with very large charge; and preconstruction R&D associated with the construction of the SLC.

The latter includes the R&D necessary to produce and accelerate bunches of electrons of appropriate intensities and low emittance, beam optics studies of the entire SLC system, and the study of particular problems associated with the final focusing of micron-size beams. Also under study and development are sources to produce and accelerate polarized electrons in high intensity bunches.

Goals and/or Major Results to Date

A program to modify the first sector of the SLAC linac to allow studies of extremely high current, single electron bunches in the linac has been under way since 1981.

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Upgrading of steering, focusing, and beam position monitoring systems in the first ten sectors of the linac, as well as instrumentation and controls for those systems, was completed (with AI funds) in FY 1982 and FY 1983. Work continued on the preinjector system providing high current, low emittance electron beams in very short bunches.

During FY 1984 further adjustments and improvements have been made on components of the injector, the damping ring system, and the linac up to Sector 10.

During FY 1985 and FY 1986, the experimental program with the damping ring and first ten sectors of the linac will continue. Construction of the second damping ring and positron source will be completed during this period under the SLC construction project, and these will be debugged and brought into operation. R&D work will continue on the laser source for producing polarized electrons. Final-focus problems will be studied to optimize effective luminosity at the interaction point. Beam position indicators for the final focus region will be developed. It is anticipated that much of the modified control system for the linac being funded under the Accelerator Improvement Program will become operational during 1986.

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Title of Project: Nuclear Physics Support

Person in Charge: L. Keller

Scientific and Professional Staff: R. Arnold, P. Bosted, R. Gearhart, A. Gomez, A. Katramatou, G. Petratos, S. Rak, A. Sill, and Z. Scalata

Scope of Work

SLAC support of the Nuclear Structure Physics experimental program to be conducted in End Station A includes all the services traditionally supplied by SLAC to its high energy physics users, including set-up and checkout of SLAC-supplied targets and detection equipment, provision of mechanical and electrical utilities, and other data-logging support. Specifically excluded from the scope of this work is direct support of experimental user groups, maintenance, and operation of experimental devices supplied by users.

Goals and/or Major Results to Date

During FY 1984 a new injector (Injector East) is being installed at the Stanford Linear Accelerator Center to deliver high intensity electron beams (13.5 to 27 microamps average current at 180 pps) in the energy range 0.4 to 2.9 GeV. The proposed experimental program includes a series of elastic and inelastic electron scattering experiments on light elements at forward and backward angles (37 to 180 degrees) to separate the longitudinal and transverse structure functions. The major emphasis will

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be on measurements at large backward angles making it possible to determine the magnetic structure functions over a large range of momentum transfers. The new data will probe the short distance region of the nucleon-nucleon interaction; will be sensitive to high-momentum components of the ground-state nuclear wave functions; and lead to a better understanding of the role of the underlying nucleon constituents (quarks) in nuclear structure.

The Nuclear Structure Physics Program will begin in FY 1985. It will use the new injector (Injector East) and the End Station A spectrometer facility for a series of elastic and inelastic electron scattering experiments at various angles to determine the magnetic functions over a large range of momentum transfers.

The nuclear structure experimental program will continue in FY 1986.

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PART II

FINANCIAL PLAN PROGRAMS

AMES LABORATORY
Ames, Iowa

Award No.: W-7405-ENG-82

Title of Project: Theoretical High Energy Physics

Person in Charge: B-L. Young

Scientific and Professional Staff: C. L. Hammer, K. E. Lassila, R. A. Leacock, T. G. Rizzo, K. L. Whisnant, and B-L. Young

Scope of Work

This group is engaged in a wide range of investigations from the phenomenological study of lepton, quark, and gluon interactions to the mathematical foundations of quantum field theories. Recent studies have concentrated on the phenomenological implications of extended electroweak gauge theories, grand unified theories, supersymmetry, and subquark models for experiments planned at LEP and SLC. These studies range from restricting the masses and couplings of right-handed neutrinos to an analysis of the anomalous magnetic moment of the muon in extended electroweak gauge theories. They are also studying Sine-Gordon and other field theories at finite temperature as well as anomalies in model field theories.

Goals and/or Major Results to Date

Recent results include (1) investigation of consistent (preon) models of quarks and leptons within the framework of grand unification and study of the CERN anomalous events; (2) detailed studies of left-right model predictions for polarized Bhabha scattering and $e^+e^- \rightarrow \mu^+\mu^-$ at TRISTAN, SLC; and LEP energies, (3) study of the possibility that right-handed currents contribute to particle decays, (4) investigation of low energy consequences of Grand Unified Theories based on the existence of a new low-mass scale in SO(10) including lepton number violations and supersymmetry; (5) calculation of the weak contribution to the muon anomalous magnetic moment in the left-right and other extended electroweak models emphasizing possible Higgs boson effects; (6) study of symmetry breaking in SO(10) and the prediction of additional W and Z bosons at intermediate energies; (7) study of quark recombination functions and fragmentation functions of heavy quarks; and (8) field theoretic study of renormalization and confinement.

Anticipated work includes (1) continued studies of composite models with emphasis on the possibility of composite gauge bosons; (2) obtaining new limits for τ substructure using e^+e^- processes; (3) obtaining constraints on the strength of right-handed current couplings of quarks and leptons and the properties of heavy Majorana neutrinos; (4) study of the phenomenology of gauge couplings of vector bosons, photons, and Higgs particles; (5) radiative corrections in extended electroweak models; (6) study of neutrino oscillations with emphasis on the three-neutrino case;

(7) study of single W production in e^+e^- annihilation; and (8) further study of confinement, jet evolution, chiral anomalies, and application of the action variable formalism developed at Ames to the study of composite gauge bosons.

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Title of Project: Experimental High Energy Physics

Person in Charge: A. Firestone

Scientific and Professional Staff: E. W. Anderson, A. Breakstone, H. B. Crawley, A. Firestone, J. M. Hauptman, J. W. Lamsa, W. T. Meyer, and E. I. Rosenberg

Scope of Work

This program emphasizes the study of the quark and gluon structure of hadronic matter. At this time, Ames is engaged in three large experimental programs: (1) Proton-proton and antiproton-proton interactions in the Intersecting Storage Rings (ISR) at CERN, using the Split Field Magnet detector. These experiments are designed to study quark and gluon jets produced at large momenta transverse to the beam axis; (2) Study of the production of high-mass muon pairs in the very forward direction in pion-nucleon interactions at Fermilab, in order to investigate the quark structure of mesons; and (3) Study of the electroweak interaction and its use as a probe of hadronic structure using the DELPHI detector being built at the CERN Large Electron-Positron (LEP) collider. Of foremost importance will be detailed studies of the vector bosons (Z^0 and W), gauge bosons (Higgs particles), heavy leptons, and new quarks, as well as studies of how the quarks and gluons materialize as hadrons. The Ames group is responsible for the design and construction of the readout electronics for the High-density Projection Chamber (HPC) electromagnetic calorimeter. The HPC is a new device based on long electron drifts which aims at complete three-dimensional imaging of electromagnetic showers with very high granularity in all space coordinates.

Goals and/or Major Results to Date

In the ISR program, Ames has (1) shown the gluon to be a vector particle; (2) measured inclusive cross sections and $K^\pm/\pi^\pm$ ratios as functions of $\sqrt{s}$ and p_T and has shown them to be consistent with the quark-gluon picture; (3) demonstrated the flavor tagging of hadronic jets in which $\pi^\pm$ and K^+ jets are quark-initiated and K^- jets are gluon initiated in pp interactions; and (4) measured $\overline{p}p$ elastic scattering differential cross section over a wide range of momentum transfers. Future goals for data currently being analyzed include measurement of the production of hadrons containing charmed and bottom quarks, and a search for gluonic bound states produced in the central region in the double Pomeron exchange reaction.

AMES LABORATORY
Ames, Iowa

In the Fermilab dimuon program, Ames is currently taking data with 75 GeV/c and 250 GeVc π^- beams at incident intensities up to 5 x 10^9 pions per second. Anticipated results include comparison of measured cross sections with the predictions of the quark-antiquark annihilation model, detailed studies of the dimuon angular distribution, extraction of the charged pion valence quark structure function, and a search for scaling violations.

In the DELPHI project at the CERN LEP Collider Ames is designing a state-of-the-art CCD-based readout electronics chain for the HPC electromagnetic calorimeter. The essential requirements are sufficient dynamic range to measure accurately both low energy showers (< 1 GeV) and the cores of the highest energy showers (> 50 GeV), high speed (< 40 nanoseconds per sample), and reasonable cost. Ames has built 64 channels of readout electronics for the full-scale prototype module, and is presently engaged in an extensive program of testing and refinement. Mass production of the 12000 electronics channels needed is expected to begin early in 1985 and data taking at LEP is expected to begin by the end of 1988.

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LOS ALAMOS NATIONAL LABORATORY
Los Alamos, New Mexico

Award No.: W-7406-ENG-36; E161

Title of Project: Elementary Particles and Field Theory (Group T-8)

Persons in Charge: G. I. Bell, P. Carruthers, and F. Cooper

Scientific and Professional Staff: Peter Carruthers, F. Cooper, D. Campbell, B. Hasslacher, M. Nieto, S. Raby, D. Sharp, R. Slansky, G. West, M. Grady, A. Kostelecky, and Y. Tosa

Scope of Work

Group members conduct research over a broad spectrum of basic particle physics and field theory. In addition to the development of new concepts, techniques and applications of quantum and classical field theory, a major effort is being made to exploit the promise of supersymmetry, supergravity, and dimensional reduction. Another major activity concerns the development of QCD in all aspects: confinement, perturbative, and stochastic evolutions. A continuing phenomenological program applies these results to jet phenomena and multiparticle productions. New developments in nonlinear dynamics, especially in conjunction with staff and visitors in the Center for Nonlinear Studies, are under scrutiny for revealing new aspects of field theory. Other significant activities include research on basic quantum mechanics and the adaptation of numerical finite element techniques to quantum field theory. Some effort is also devoted to the study of new facilities issues relating to the SSC, LAMPF II, and the proposed National Underground Science Facility.

Goals and/or Major Results to Date

Significant results have been obtained recently in many areas. A supersymmetry theory (finite to at least two loops) has allowed the prediction of fermion masses, in particular, the top quark mass at about 150 GeV. In an improved lattice calculation of SU(2) gauge theories, a critical point was found in a noncompact theory, implying that neither formulation of SU(2) lattice gauge theory confines in the continuum limit. A new stochastic formulation of multiparticle production has produced a successful and suggestive explanation of KNO scaling in multiparticle production. Several new calculational techniques for field theory have been formulated and are being subjected to further tests.

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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts

Award No.: DE-AC02-76ER03069

Title of Project: Counter Spark Chamber Group

Persons in Charge: W. Busza, J. I. Friedman, H. W. Kendall, V. Kistiakowsky, L. S. Osborne, L. Rosenson, and F. E. Taylor

Scientific and Professional Staff: W. Busza, J. I. Friedman, H. W. Kendall, V. Kistiakowsky, L. S. Osborne, L. Rosenson, J. S. Whitaker, and F. E. Taylor

Scope of Work; Goals and/or Major Results to Date

1. The construction and use of a novel fine-grained high-mass neutrino detector for the study of the nature of weak interactions, the structure of nucleons, and search for new neutrinos.
2. The design and construction of a facility at Fermilab for the study of muon scattering at Tevatron energies. Studies with this facility will include nucleon structure functions and quark fragmentation.
3. The design and construction of a very high-resolution detector (SLD) to be used at the Stanford Linear Collider for the study of the production and decay of the neutral weak vector boson, Z^o.
4. The construction and operation of a large solid angle detector for photons and charged particles, to be used at PEP in search for electron-positron annihilation yielding only "non-interacting" particles.

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Title of Project: Accelerator Physics Collaboration APB - Bubble Chamber Program

Person in Charge: I. A. Pless

Scientific and Professional Staff: E. S. Hafen, R. I. Hulsizer, I. A. Pless, and R. K. Yamamoto

Scope of Work; Goals and/or Major Results to Date

The APC is engaged in the continuation of last year's efforts. Last year it closed out the work on the 8 GeV/c SLAC efforts. This year it is contemplating adding a new effort on high energy, high multiplicity events induced by the interactions of hadrons with nuclei. A proposal was submitted in collaboration with Tohoku University, and others, to do a mu-neutrino experiment (E745) in conjunction with the test run for E636. This proposal was approved and scheduled to run at Fermilab in December 1984.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts

The list of topics that concern the APC are:

1. $(\pi^+, K^+, p) + p$ at 147 GeV/c:

This experiment (FNAL E299) is in the analysis stage. This work is being done in collaboration with members of the International Hybrid Spectrometer Consortium (IHSC). The main point of study is the dependence of interactions on the quantum numbers of incident particles.

2. $(\pi^+, K^+, p, \pi^-) + p$ at 200 GeV/c:

This experiment (FNAL E570) is currently being run in collaboration with the IHSC. It utilizes the FNAL hybrid spectrometer with a new downstream Particle Identifier (DPI) based around CRISIS and a new High Resolution Optics (HRO) camera. This will enable the study of charmed particle production, as well as the production of particles with specific quantum numbers, as a function of incident particle.

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Title of Project: Electromagnetic Interactions Group (EMI)

Person in Charge: S. C. C. Ting

Scientific and Professional Staff: U. J. Becker, J. Branson, J. D. Burger, M. Chen, P. D. Luckey, and S. C. C. Ting

Scope of Work

The Electromagnetic Interactions Group is currently involved in two major projects involving international collaborations. The EMI group bears the major responsibility for the design, construction, assembly, execution, and data analysis of all its experiments.

1. The PETRA accelerator at DESY, Hamburg, Germany is currently scanning up to 46 GeV. Thus, it is the highest energy e^+e^- accelerator in the world. The MARK-J Experiment has been designed to measure μ, $\mu\mu$, ee and hadron jets precisely and is distinct from the other PETRA detectors. Among its physics goals are the following:

   a. search for top quark up to $\sqrt{s} \approx 45$ GeV;
   b. measure the $\mu^+ \mu^-$ charge asymmetry and study Z^0 propagator effects;
   c. search for new leptons, supersymmetric scalar particles;
   d. study QCD jets

During 1983 MARK-J has gathered data at the highest available energies and has yielded physics results on a range of topics.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts

MIT has continued its search for the top quark and has tested models without the top quark. They have conducted precise measurements on a model independent second order determination of the strong coupling constant α_S and carried out studies on inclusive muon spectra from the electron-positron collisions at the highest PETRA energy regions. In 1984 MIT expects to extend the search for new particles. They also plan to upgrade the MARK-J detector by installing a Time Expansion Chamber prototype of the LEP vertex chamber as well as the first production of BGO from LEP-3. This will give significant improvements in detector performance as well as allow them to debug the detector, data collection, and analysis systems in advance of the start up of LEP scheduled for 1988.

2. The approved LEP-3 experiment at the LEP accelerator at CERN, Geneva, Switzerland is now in construction phase. This effort is proceeding under a tight schedule to meet the first LEP beam. The main interest in LEP is to study and search for new phenomena at $\sqrt{s} = 180$ GeV in the first stage and 10 TeV $\overline{p}p$ in the second stage which is scheduled for the early 1990's. MIT's detector is unique and distinct from the other three LEP experiments. Among the distinct features are the following:

   a. Measurement of photons, electrons, and muons with a resolution of $\Delta p/p = 1$ percent.

   b. Measurement of hadron jet energies with a good resolution together with leptons.
   c. Precision measurement of vertices.
   d. The large magnetic hall with a $BL^2 = 160$ kG-m^2 and the fact that the central part of the detector can be easily modified or removed, making this experiment readily adaptable for future phases of LEP.

   In the technical design of this experiment; every effort has been made to ensure that the resolution of detecting photons, leptons, and hadron jets is optimized. The physics is a logical continuation of the work being done over many years at DESY, BNL, and the ISR.

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Title of Project: Particle Theory

Person in Charge: J. Goldstone

Scientific and Professional Staff: E. Farhi, D. Freedman, R. Giles, A. Guth, K. Huang, R. Jackiw, R. Jaffe, A. K. Kerman, K. Johnson, and V. F. Weisskopf

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts

Scope of Work; Goals and/or Major Results to Date

As for the past few years research is focused on the structure and application of gauge field theories in the following areas:

1. non-perturbative structures in field theories, especially those related to topological properties.
2. models of particles and interactions, including supersymmetric theories.
3. cosmological consequences of grand unified gauge theories, especially the inflationary scenarios for the very early universe.
4. quantum chromodynamics (QCD) as a theory of strong interactions, including computer studies of lattice QCD.
5. QCD applied to analysis of experiments, including those of heavy nuclei.

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Title of Project: Optics for a Spin-Polarized Hydrogen Atomic Beam

Person in Charge: D. Kleppner and T. Greytak

Scientific and Professional Staff: none

Scope of Work; Goals and/or Major Results to Date

MIT is developing cryogenic techniques of producing polarized protons for use in targets, jets, and sources. These techniques follow from success in producing high densities of electron and nuclear polarized atomic hydrogen gas at temperatures below 0.3K. They are collaborating with a group at Brookhaven (Alan Krisch) on the design of a cold jet of nuclear polarized atomic hydrogen for use in the AGS. MIT is studying the production of solid nuclear polarized modecular hydrogen.

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OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee

Award No.: DE-AC05-84OR21400

Title of Project: High Energy Accelerator Shielding Studies

Person in Charge: R. G. Alsmiller, Jr.

Scientific and Professional Staff: R. G. Alsmiller, Jr., T. A. Gabriel, and R. L. Lillie

Scope of Work

The purpose of the program is to use the best available cross-section data and radiation transport methods to provide calculated design data to aid in the design of the shielding for high energy accelerators. Calculated design data are also provided to researchers who are engaged in the design of instrumentation (calorimeters) and to investigators to aid in the interpretation of their experimental data. Investigators often prefer to perform their own calcualtions with the computer codes developed under this program. When this is the case, every effort is made to install the computer codes on the investigators' computing equipment and to familiarize them with the use and operation of the codes.

To ensure that the supplied data are as accurate as possible, a part of the program is directed at obtaining comparisons between calculated results and the latest available experimental data.

The accuracy of transport calculations is dependent upon the differential particle-production cross-section data that are used, as well as on the transport methods employed, and, therefore, studies in both of these areas are included in the program. In general, however, requests for design data are always given precedence over methods development.

Goals and/or Major Results to Date

1. To supply at the request of high energy physics researchers, state-of-the-art calculated radiation transport data in the areas of shielding, instrumentation design (calorimeters), experimental setup, and data interpretation.
2. To maintain close communication with investigators so that important feedback information can be incorporated into future calculations.
3. To document and distribute data and calculational techniques for ready availability to all researchers.

Data provided by this program have been used to design the shielding of almost all of the accelerators constructed in the United States in the past 20 years. Calorimeters designed on the basis of results obtained as part of this program are in use at FNAL, SLAC, BNL, and CERN.

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OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee

Title of Project: High Energy Physics

Person in Charge: H. O. Cohn

Scientific and Professional Staff: J. E. Brau, W. M. Bugg, H. O. Cohn, G. T. Condo, and T. Handler

Scope of Work

Experimental elementary particle physics is pursued with hybrid bubble chamber techniques, however, the program is shifting from reliance on bubble chamber techniques to counter experiments. Studies of charm photoproduction in the SLAC 40" hybrid bubble chamber with high resolution optics is nearing completion. Hadron and strange particle production are also studied in these experiments. Analysis of slow antiproton interactions with nuclei have been performed in light of the renewed interest of this subject resulting from interpreting proton decay results in $n\bar{n}$ oscillation limits and speculation on the subject of quark-gluon plasma. Preparations are also under way for a search for the elusive tau neutrino in a beam dump experiment with the Tevatron at Fermilab. A precursor experiment will study charm production and other short lived particles and test the equipment for the ν_τ experiment.

Goals and/or Major Results to Date

Lifetimes and cross sections for charged and neutral charmed particles produced in 20 GeV γp interactions have been measured. A limit has been set on the magnitude of the "contact term" in a run near threshold for charm photoproduction. They have measured $\bar{p}$ cross sections with carbon and lead at 70 MeV and obtained values for Λ production and a limit on the dibaryon production in $\bar{p}$ nucleus reactions. Their goal is to observe the tau neutrino and to study properties of charmed particles. They also will participate in the SLD development and subsequent physics at SLC.

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PACIFIC NORTHWEST LABORATORY
Richland, Washington

Award No.: AC06-76RL01830

Title of Project: Ultrasensitive Investigation of Neutrinoless and Two Neutrino Double Beta Decay of ^{76}Ge

Person in Charge: R. L. Brodzinski

Scientific and Professional Staff: D. P. Brown, J. C. Evans, Jr., W. K. Hensley, J. H. Reeves, and N. A. Wogman. (F. T. Avignone, III, from the University of South Carolina is also a co-investigator but does not receive any DOE-HEP funding.)

Scope of Work

The objectives of this research program are to determine the neutrinoless and two-neutrino double beta decay rates of ^{76}Ge to the ground state and 2+ first excited state of ^{76}Se. The approach is to design and fabricate a multicrystal germanium diode gamma-ray spectrometer from materials having nonmeasurable concentrations of radioactive contaminants and to locate this spectrometer system at the 4850 foot level in the Homestake Gold Mine in Lead, South Dakota, in order to minimize the effects of cosmic radiation. The high resolution, ultra-low-background investigation allows decays to the ground state and excited states of the daughter nuclide to be distinguished from one another. In addition, a natural byproduct of the double beta decay investigation is a higher sensitivity search for spontaneous electron decay. The purpose of the program is to acquire high quality data concerning the neutrino mass and the level of lepton conservation, both of which provide valuable tests of Grand Unified Theories. The projected sensitivity limits of the large detector for the ^{76}Ge neutrinoless ground-state double beta decay half-life, neutrino mass, and weighting of the right handed neutrino current are $T_{1/2} \geq 2.6 \cdot 10^{24}$ y, $m_\nu \leq 0.6$ eV, and $\eta \leq 2 \cdot 10^{-6}$.

Goals and/or Major Results to Date

Radiopure materials for fabricating the large multicrystal germanium spectrometer have been identified. A prototype spectrometer has been fabricated from these materials and installed in a large lead shield in the Homestake Mine. After more than 76,000 minutes of data accumulation, absolutely no manmade or primordial radioactivity has been found in the detector assembly. The system background is more than an order of magnitude lower than ever achieved anywhere else in the world. A new limit on the ^{76}Ge neutrinoless double beta decay rate has been measured. The first of the two seven-crystal arrays has been assembled and is undergoing testing.

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UNIVERSITY OF ALABAMA
Tuscaloosa, Alabama

Award No.: DE-FG-05-84ER40141

Title of Project: Comprehensive Study of ψ-Meson Production

Persons in Charge: B. C. Harms and S. T. Jones

Scientific and Professional Staff: B. C. Harms and S. T. Jones

Scope of Work; Goals and/or Major Results to Date

The objective of this work is to study the various processes by which ψ mesons (charmonium) and other bound states of heavy quarks (quarkonium) are produced. This study consists of perturbative calculations in the presently accepted gauge theory of strong interactions, quantum chromodynamics (QCD). The purpose of the calculations is to obtain predictions of differential and total cross sections or decay rates. The comparison of these quantities with experimental data constitutes an important test of QCD and of the model used for the bound states of heavy quarks.

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PART III

UNIVERSITY PROGRAMS

UNIVERSITY OF ARIZONA
Tuscon, Arizona

Award No.: DE-AC02-80ER10663

Title of Project: High Energy Physics

Person in Charge: K. W. Lai

Scientific and Professional Staff: L. R. Cormell, M. V. Arenton, W. Dieterle, and K. W. Lai

Scope of Work

The group's primary activity is to search for and study charm and beauty particles produced by hadronic interactions at Fermilab using a new and different approach (E580 and E623). In addition, they are also engaging in a unique jet experiment (E683) by using the photon beam at Fermilab as an important part of the extension of studies of jet production by hadrons (E609).

Goals and/or Major Results to Date

The most recent major results are observations of the charmed D and F particles as well as candidates for beauty particles at Fermilab. In the future, they will be using the E705 spectrometer to study further beauty particles with 300 GeV/c π^- and $\overline{p}$ beams, and a plan is under way to construct a large hadron calorimeter for E705 in order to select beauty events with good efficiency. This hadron calorimeter will also be used for E683 to obtain better coverage of the jets from photoproduction. The group will play a leading role in E705 as well as E683.

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Title of Project: Theory and Phenomenology of High Energy Physics

Persons in Charge: M. D. Scadron, R. L. Thews, and A. Patrascioiu

Scientific and Professional Staff: Same as above

Scope of Work

The members of this group all perform basic theoretical physics research in various areas of high energy physics. Topics currently under investigation range from formal topics such as dynamical mass generation in quantum field theory and nonlinear dynamics in classical statistical mechanics, to phenomenological studies of chiral symmetry breaking in QCD, weak decays of quarks, spin structure of hard scattering processes for constituent models, and extraction of quark distribution functions from high energy collision data.

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UNIVERSITY OF ARIZONA
Tuscon, Arizona

Goals and/or Major Results to Date

An interesting example of nonequipartition of energy has been found for some classical nonlinear systems. Work has been completed on a comprehensive description of particle mixing for all strong and electromagnetic processes, including the charmed sector, for all meson nonets. A description of all nonleptonic decays of hyperons has been achieved.

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BOSTON UNIVERSITY
Boston, Massachusetts

Award No.: DE-AC02-83ER40118

Title of Project: Field Theoretic Investigations on Particle Physics and Cosmology

Person in Charge: S. Y. Pi

Scientific and Professional Staff: S. Y. Pi

Scope of Work

The main research effort concerns the impact of particle physics on early universe cosmology. More specifically, the program is to study various aspects of the "Inflationary Universe". The inflationary scenario for the early universe provides possible answers to some of the fundamental problems in the standard cosmology--the flatness, horizon, and monopole over-abundance problems. The idea involved in the inflationary universe is simple and, therefore, attractive. The key features are the following: 1) There was a period of exponential expansion in the early universe, called "inflation"; and 2) Our universe has emerged from a region, called a "fluctuation" region, whose radius is smaller than the horizon distance. However, there are difficulties in realizing this idea in particle physics. Various detailed field theoretic studies to understand and overcome the difficulties and also to construct a realistic inflationary particle physics model will also be conducted.

Goals and/or Major Results to Date

1. A most remarkable consequence of the inflationary universe is that although it was not designed to do so, it can provide an answer to an important cosmological puzzle--the origin of initial inhomogeneities which led to galaxy formation. In the inflationary picture, quantum fluctuations which occurred during inflation give rise to the initial inhomogenities--the fluctuations in the energy density. Together with A. Guth, she calculated the spectrum of density fluctuations predicted by the inflationary universe, and found that the density fluctuations have the desired scale invarient Zeldovich spectrum, but their magnitude is about 10^5 times too large in the standard SU(5) model with the Coleman-Weinberg potential. The result is important in that the magnitude of density fluctuations consistent with observation puts a strong constraint on the inflationary model building.

2. Together with A. Guth, a detailed field theoretic analysis has been performed on the phase transition which is required by the "new" inflationary universe---the most popular version of the inflationary scenario. They have established the validity of some of the important assumptions involved in the scenario.

3. A realistic inflationary particle physics model in which all the cosmological constraints are satisfied has been constructed.

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BOSTON UNIVERSITY
Boston, Massachusetts

Title of Project: Field Theoretic Investigations on Particle Physics and Cosmology

Person in Charge: A. Yildiz

Scientific and Professional Staff: S. Ben-Menahem, W. Hellman, and A. Yildiz

Scope of Work

The group pursues research in selected areas of Theoretical High Energy Physics and Cosmology. A program for visiting theoreticians from abroad and the United States has been instituted. In addition to the Boston Area Physics Calendar Colloquia, a new TABU (Theory at Boston University) weekly seminar series was established last year and continues. The seminars concern recent theoretical and experimental topics that are closely related to the group's program. Also the group is involved in the organization of the Grand Unification Workshop series which are held at different institutions.

Goals and/or Major Results to Date

During the past year, the group produced important and relevant results in Particle Physics and Cosmology and Esoteric Field Theories; including hypercolor unification without cosmological domains, heavy quarkonia systems with a new color force to explain anomalous events of the $p\bar{p}$-collider experiments. Also, a finite temperature formalism that maintains Lorentz covariance is used to investigate finite temperature corrections to the electron mass, electron magnetic moment and vacuum energy. The group's continuing research activities include the phenomenology of the ongoing experiments in the U.S. and abroad, and the unification and relevant symmetry related to field theories.

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BRANDEIS UNIVERSITY
Waltham, Massachusetts

Award No.: DE-AC02-76ER03230

Title of Project: Experimental High Energy Physics

Persons in Charge: L. E. Kirsch and J. R. Bensinger

Scientific and Professional Staff: L. Spencer and H. Piekarz

Scope of Work

The group is currently performing two experiments. The first is a study of weak hyperon radiative decays at the MPS spectrometer at Brookhaven using a lead glass array. The goal of this experiment is to determine the nature of the quark interactions which contribute to the weak decay process.

The second project is a contribution to the international collaboration building the Colliding Detector Facility at Fermilab. This will be the primary detector for the Tevatron I antiproton-proton collider, which will explore this new energy regime.

Goals and/or Major Results to Date

The radiative decay experiment has completed data acquisition, and is presently in the analysis stage. They expect to be able to measure the asymmetry parameter for the cascade radiative decay.

The group, along with Harvard, is responsible for construction of the electromagnetic shower calorimeters for the CDF project. Studies have also been completed for trigger methods utilizing these calorimeters.

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Title of Project: Theory

Persons in Charge: L. F. Abbott and H. J. Schnitzer

Scientific and Professional Staff: L. F. Abbott, H.-Y. Cheng, R. Flores, and H. J. Schnitzer

Scope of Work

The Brandeis High Energy Theoretical Physics Group pursues research in quantum field theory, elementary particle phenomenology and cosmology. A major part of this research deals with meson spectroscopy, composite models, Skyrmions, the cosmic microwave background, the background field method, quantum gravity and C. P. violation. In addition, members of the theory group have close contact with the Brandeis experimental group and participate in joint seminars and discussions. They also have frequent contact with other members of the greater Boston high energy physics community through informal discussions and a formal weekly seminar.

BRANDEIS UNIVERSITY
Waltham, Massachusetts

Goals and/or Major Results to Date

During FY 1985 members of the Brandeis High Energy Theoretical Physics Group hope to extend their work in a variety of research topics: meson spectroscopy, composite models, Skyrmion models, cosmology, quantum gravity, early universe, and galaxy formation. These research topics cover a broad spectrum of the frontier areas of particle physics.

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BROWN UNIVERSITY
Providence, Rhode Island

Award No.: DE-AC02-76ER03130

Title of Project: High Energy Theory

Persons in Charge: H. M. Fried

Scientific and Professional Staff: D. Feldman, H. M. Fried, A. Jevicki, K. Kang, and C-I. Tan

Scope of Work

Studies span most of the modern theoretical topics of high current interest, plus a few which may become important in the near future. While continuing his work on loop-space correlations in QCD, A. Jevicki and students are setting up a computer formulation of quantum gravity and various models of supersymmetry. A very thorough elaboration of possible grand unification theories possessing certain desirable properties, in agreement with the recent results of proton decay experiments, has been performed by K. Kang and associates, with direct applications to modern cosmology. Studies of General Relativity and Group Theory, in particular the relevance of very general group contractions in Kaluza-Klein-like theories, has been under investigation by D. Feldman. Understanding lattice gauge theory has been the principal recent topic of C-I Tan and associates, in a series of papers devoted to a practical modeling of QCD-like theories; recently, in collaboration with M. Ninomiya, difficulties with the SLAC Lagrangian were analyzed. Studies of strong-coupling approximations to quantum field theories by the method of infrared extraction have been the principal study of H. M. Fried, along with relevant approximations to ordered exponentials and to the generation of turbulence in Navier-Stokes theory. M. Ninomiya and collaborators have continued their studies of "no-go" theorems in lattice QCD; and have worked with C-I Tan on lattice quantization. They are presently studying general axial anomalies with A. Jevicki. S. Libby and collaborators have produced a solution to the quantum Hall effect, of great importance to both solid state physics and to the understanding of the role of the QCD θ-parameter and the smallness of CP violations in high energy physics.

Goals and/or Major Results to Date

General goals include: the understanding and development of lattice quantization for QCD and quantum gravity with and without supersymmetry; the specification of possible grand unified theories and their predictions for modern cosmology; and alternative strong-coupling, continuum techniques for QCD and other field theories. Some major results to date include: definitive restrictions on possible grand unified theories and on the choice of certain lattice Lagrangians; two strong-coupling approximations for SU(2) ordered exponentials; and a new, fundamental explanation of the quantum Hall effect.

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BROWN UNIVERSITY
Providence, Rhode Island

Title of Project: Bubble Chamber/Hybrid

Person in Charge: M. Widgoff

Scientific and Professional Staff: D. Brick, A. Shapiro (on leave at DOE), and M. Widgoff

Scope of Work

They have two new experiments in preparation and two in the stage of data analysis. The group is preparing for two approved Tevatron II experiments: E636, a search for the tau neutrino using a beam dump as source, is scheduled to run in 1986, with a test of the bubble chamber-hybrid detector system to be carried out in the winter of 1984-85. This test will provide the data for E745, a study of interactions in a muon neutrino beam at high energies. The target of the new hybrid system is a one-meter bubble chamber photographed holographically to give the high resolution needed to detect close decays: the system includes trigger counters, drift chambers, a muon detector and CRISIS for particle identification by ionization sampling. The group at Brown is building scintillator hodoscopes for the trigger. They are analyzing data from two other experiments (FNAL and SLAC), both done with hybrid systems. One is a study of hadron interactions at 200 Gev/c as a function of beam particle quantum numbers (π^+, K^+, p), and of target atomic weight (H, Mg, Ag, and Au): the other is a study γp interactions at 20 GeV, including photoproduction of charmed particles.

Goals and/or Major Results to Date

Goals are the completion and testing of the detectors needed for the neutrino experiments at the Tevatron; the test of the new hybrid system which will provide the data for the experiment on muon neutrino interactions, as well as giving preliminary information needed for the beam-dump tau neutrino study; and the carrying out of the latter experiment starting in 1986. Meanwhile they expect to be learning interesting physics from the hadron and photon experiments. A number of papers and talks have been published both on various aspects of hadron interactions and on the photoproduction of charm, strange particles, and vector mesons.

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Title of Project: Electronic Detector Group

Person in Charge: R. E. Lanou

Scientific and Professional Staff: D. Cutts, J. Hoftun, J. T. Massimo, and T. Shinkawa

BROWN UNIVERSITY
Providence, Rhode Island

Scope of Work

The work of this group centers on two major projects. One, being conducted at the BNL-AGS, is a second generation study of weak, neutral current phenomena. It measures the elastic scattering of neutrinos (and anti-neutrinos) from electrons and protons. The aim is to measure as precisely as possible the fundamental parameters, sin $^2\theta_w$ and rho, of the Standard Model as well as to determine model independent couplings. The experiment makes use of the large neutrino detector of a new type constructed by this collaboration. Additional results are aimed for in the area of neutrino mass phenomena such as neutrino oscillations using the same detector. A second project involves the carrying out (and construction of a detector to do so) of a new experiment (E740) at the Tevatron I of FNAL (D-Zero Project). This experiment aims to search for new phenomena occurring at the highest energy and luminosity available (2 TeV and 10^{30} cm^{-2} sec^{-1}) and to test the validity of theories in this new, physical regime.

Goals and/or Major Results to Date

Goals in the next period center upon additional accelerator running for the neutrino experiments, completion of analysis of present data, and initiation of research and development in the areas of transition radiation and high speed data acquisition hardware for the D-Zero project. Recent results presented in publications and at physical society meetings have concerned neutrino (and anti-neutrino) cross sections on electrons, limits on muon-type neutrino mixing to electron-type neutrino, and limits on magnetic monopole fluxes at sea level.

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UNIVERSITY OF CALIFORNIA, BERKELEY
Berkeley, California

Award No.: DE-AT03-84ER40161

Title of Project: High Energy Physics and Cosmology

Persons in Charge: J. Silk, and S. White

Scientific and Professional Staff: J. R. Bond, M. Davis, N. Kaiser, and A. Szalay

Scope of Work

This research effort focuses on the implications of recent theories and experiments in high energy physics for the evolution of the early universe, and on the constraints that cosmological considerations can place on such theories. Several problems are under investigation, including developing constraints on the inflationary predictions of scale-free primordial flunctuations in a universe at critical closure density by studying their linear evolution after they reenter the particle horizon, the formation and possible fragmentation of large-scale anisotropic structures whose dynamics are dominated by massive weakly interacting particles such as massive neutrinos or photinos (this will model the formation of galaxies, galaxy clusters, and superclusters), and the observable imprint of the adiabatic density fluctuations predicted by GUTs on the cosmic microwave background radiation. They expect such astrophysical considerations to provide fruitful insights both into high energy particle physics and into possible cosmological models for the early universe.

Goals and/or Major Results to Date

It has been shown that astrophysical constraints, including those from numerical simulations of the galaxy correlation function and from the dipole anisotropy of the cosmic microwave background radiation, are incompatible with the conventional neutrino-dominated cosmology. A stable neutrino rest mass cannot exceed a few eV; other particles must dominate the non-density of the universe.

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UNIVERSITY OF CALIFORNIA
Davis, California

Award No.: DE-AT03-76ER70191

Title of Project: High Energy Particle Physics

Person in Charge: R. Lander

Scientific and Professional Staff: W. Ko, R. Lander, D. Pellett, J. R. Smith, J. Volk, W. Wagner, and P. Yager

Scope of Work

The group studies elementary particle interactions at high energies. Past work has focussed on inclusive interactions. Present focus is on charm and beauty decay properties and photon-photon interactions at the SLAC electron-positron collider. The latter data are expected to yield theoretically "clean" information on quark dynamics. For example, the strong coupling constant can be estimated from the photon structure functions and their Q^2 evolution. High P_T jet cross sections can help to define the extent to which gluon effects, higher twist, etc., modify the simple Born interaction picture. The photon-photon partial widths can help to define the gluon content of resonances, and the total hadronic cross section (at very low Q^2) distinguishes between integer- and fractional-charge quarks. Understanding of nonperturbative QCD can be improved by low Q^2 photon-photon interactions data. The charm and beauty experiment (E653) will provide lifetimes and branching ratios. These will help determine the nature of the charm and beauty quark interactions.

Goals and/or Major Results to Date

The goals are (as outlined under "scope" above): Structure functions, total cross section vs $S_{\gamma\gamma}$, $d\sigma/dp_T^2$ for jets, particle-antiparticle pair production, and "soft" $\gamma\gamma$ interactions; also lifetimes and branching ratios for charm and beauty. Preliminary results include leptonic structure functions F_2 and F_1, Q^2 dependence of resonance production, the total cross section, and the first observation of the phi meson production in photon-photon interactions.

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Title of Project: Theoretical High Energy Physics

Person in Charge: J. Gunion

Scientific and Professional Staff: J. Gunion and J. Kiskis

UNIVERSITY OF CALIFORNIA
Davis, California

Scope of Work

The two theorists pursue research (sometimes in collaboration with graduate students) in various areas of theoretical high energy physics. Included are investigations in the areas of quantum chromodynamics (perturbative and nonperturbative), spontaneously induced gravity and phenomenology for super collider energies. In addition to regular theoretical and journal club seminars a high energy group meeting of the theoretical and experimental staff and students is held every other week in which phenomenological and other issues of general interest are discussed.

Goals and/or Major Results to Date

During FY 1983, a number of publications in perturbative and nonperturbative quantum chromodynamics (QCD) were produced which explore progress made in: 1) understanding "higher-twist" phenomena in deep inelastic scaling and high-p_T particle production; 2) higher order corrections to jet calculus decay functions including the resolution of a long standing discrepancy in the gluon sector; and 3) field configuration regularities in lattice QCD calculation of quark confinement. In addition a large number of phenomenological calculations relevant to the proposed 40 TeV super collider were performed for presentation to the $\bar{p}p$ workshop in Chicago during February 1984.

These and other topics continue to be of importance to future investigations. They impinge upon our understanding of the structure of matter and the nature of interactions between elementary particles at the most fundamental level.

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UNIVERSITY OF CALIFORNIA INTERCAMPUS INSTITUTE
La Jolla, California

Award No.: AT03-76ER70285

Title of Project: Intercampus Institute for Research at Particle Accelerators

Person in Charge: D. Caldwell

Scientific and Professional Staff: D. Caldwell, R. Lander and G. Masek; A. Eisner, B. Magnusoh, and M. Sullivan (SLAC)

Scope of Work

The Intercampus Institute for Research at Particle Accelerators (IIRPA) is an organization set up to help the research work at SLAC of the Davis, San Diego, and Santa Barbara campuses of the University of California. So far, that has meant helping to perform the PEP-9 experiment on two-photon annihilation. The current Director of IIRPA is David Caldwell (USCB), the Associate Directors are George Masek (UCSD) and Richard Lander (UCD). Scientific personnel based at SLAC are Alan Eisner, Bruce Magnuson, and Michael Sullivan.

The PEP-9 experiment is the only one in the world designed specifically to do two-photon (2γ) physics; i.e., the observation of the particles emerging from the collision of two virtual photons which result from the glancing collision of the counter-rotating electrons and positrons in the accelerator. PEP-9 is able to measure (tag) the scattered e^- and/or e^+, whereas other running experiments do 2γ physics with no tag, and hence their results are not so complete or accurate.

Mainly because the forward-backward apparatus of PEP-9 is used with the central detector of PEP-4, and the latter has both been slow to turn on and has had severe problems, PEP-9 has had very little effective running so far. However, the analysis of some data is nearing completion, and they already have published work on the electromagnetic structure function of the photon. Nearing publication are results on the double-tagged $\gamma\gamma$ total cross section, the hadronic structure function of the photon, zero-tag and single-tagged production of various resonances (η, η', f^0, A_2) to measure their 2γ widths and the Q^2 dependence of their production, and the study of the 4π and $\pi\pi K\bar{K}$ production, giving information on enhancements which may be the first evidence for four-quark states of matter.

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UNIVERSITY OF CALIFORNIA
Irvine, California

Award No.: DE-AT03-76ER71019

Title of Project: Research Program in Neutrino Physics, Cosmic Rays, and Elementary Particles

Person in Charge: F. Reines

Scientific and Professional Staff: R. Allen, H. Chen, P. Doe, W. Gajewski, K. Ganezer, R. Greenwood, A. Hahn, W. Kropp, M. Moe, L. Price, H. Sobel, and K. Wang

Scope of Work

The group is investigating problems in low and intermediate energy neutrino physics including neutral current interactions of $\overline{\nu}_e$, $\overline{\nu}_e$ oscillations and double beta decay. They are collaborating in the search for baryon non-conservation (Irvine/Michigan/Brookhaven) and in the DUMAND project. Studies are in progress on the development and application of liquid Argon time projection chambers.

Goals and/or Major Results to Date

Results thus far obtained by IMB include lower limits on $p \rightarrow e^+\pi^0$ ($\tau/B >$ 2×10^{32} yrs 90% C.L.), n-$\overline{n}$ oscillations, other p and n decay modes, monopoles, and atmospheric ν fluxes. The feasibility of liquid Argon TPC detectors has been demonstrated and scaling to larger detectors is under way. The search for ν_e oscillations using fission reactors is in process at Savannah River. A gaseous TPC designed to detect ^{82}Se double beta decay is being turned on.

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Title of Project: High Energy Physics Studies

Persons in Charge: J. Schultz and M. A. Mandelkern

Scientific and Professional Staff: D. Schultz, L. R. Price, R. Ray, and T. Usher

Scope of Work

The major effort of the group is the study of the interactions of low energy antiprotons, with the specific aim of searching for baryonium and/or low mass bound and resonant states in the $N\overline{N}$ system. The most recent completed experiment is E-701 (BNL-AGS) which explored $\overline{p}d$ interactions in a search for bound and resonant states via recoil nucleon detection, and also measured the annihilation cross section ($\overline{p}p$) in the "S" region around 500 MeV/c. The current experiment is PS 183 (CERN-LEAR) which is a search for bound $\overline{P}N$ states via detection of emission gamma, pion and kaon resonances. PS 183 is based on a gamma pair spectrometer capable of

1 percent energy resolution, which also has the capability of measuring pion and kaon momenta to 1 percent, and distinguishing π's from K's. The system includes large PWC's (built at UCI), drift chambers for high precision trajectory measurements, a counter array for annihilation multiplicity, and a high speed data acquisition system capable of writing more than 100 events/sec to tape and of on line processing of several hundred/sec. Installation was completed in late 1983 and a first data run was made in December in which ten 1000 sec "shots" were received. Extensive running will be performed in the spring and summer of 1984.

Goals and/or Major Results to Date

Neutron recoil and proton recoil spectra were obtained which do not demonstrate statistically significant effects corresponding to bound states or resonances at the level of 10^{-3}/annihilation. No enhancement in the $\bar{p}p$ annihilation cross section was observed near 500/MeV/c with upper limit of 12 mb/MeV in contrast to results from some previous experiments. PS 183 preliminary data demonstrate a very significant peak in the $\pi\pm$ spectrum which would imply a bound state at ~ 1620 MeV/c^2.

There are less significant effects as well in the charged particle data. Running during 1984 will increase the data sample by more than a factor of 10 to more than 10^9 annihilations in the target, which will statistically clarify the preliminary effects. During the 1984 run, data will be collected for the processes of single meson and gamma emission; multiple meson triggers will be attempted. Two gamma running may be attempted to demonstrate the annihilation into two π^0's. An upgrade of PS 183 is under consideration in which a large fraction of the solid angle would be instrumented with gamma ray detectors. They would be able to reconstruct annihilation π^0's and thus reject that background from the gamma spectrum. Another suggestion under consideration is to place the target within a 4 π magnetic spectrometer to elucidate the decay properties of state(s) detected by the high resolution single arm spectrometer. It is anticipated that an upgrade will be implemented after September 1984 in preparation for data taking during 1985.

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UNIVERSITY OF CALIFORNIA
Irvine, California

Award No.: DE-AT03-81ER40043

Title of Project: Collective Focusing Ion Accelerator

Persons in Charge: A. Fisher and N. Rostoker

Scientific and Professional Staff: A. Fisher, N. Rostoker, F. Golden, and G. Roberts

Scope of Work

They investigate physical and technological problems associated with a compact ion accelerator. The accelerator is based on the principle of the Gabor lens; the focal length of lens for ion beams can be reduced by a factor of about 10^3 if the magnetic field confines electrons which focus the ion beam, compared with using the magnetic field directly. A toroidal cyclic accelerator experiment has been constructed; the toroidal magnetic field is produced by a discrete set of coils so that the magnetic field forms a set of weak mirrors around the torus. Electrons are confined to single mirror cells thus forming a series of Gabor lenses. A toroidal electric field is produced inductively as in a Betatron. The motion of electrons is adiabatic so that acceleration around the torus is prevented by the magnetic mirrors. The motion of ions is non-adiabatic so the electric field will accelerate them without accelerating electrons.

The major problems encountered thus far are the technology of electron injectors, the physical processes involved in injecting and trapping electrons, and stability of confined electron clouds. They also try to develop inexpensive flash-board ion sources.

Goals and/or Major Results to Date

Electrons have been injected and trapped in 16 mirror cells of a toroidal accelerator. With an applied toroidal field, less than .5 percent of the electrons were accelerated. The major physical problem was that the electron clouds vibrate at 1-10 MHz with substantial amplitude. The oscillations have the properties of the diochotron mode previously analyzed for an infinite cylinder. They have succeeded in damping this oscillation with resistive walls and have developed a new theory to explain the result. (According to the published literature, this mode is a negative energy mode which is destabilized by dissipation.) They need to develop (or buy) and characterize a suitable ion source and upgrade various experimental systems. Then experiments on trapping accelerating ions will start. The goal is to learn how to accelerate large currents of ions.

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UNIVERSITY OF CALIFORNIA
Los Angeles, California

Award No.: DE-AT03-81ER40024

Title of Project: Research in High Energy Physics (Experimental)

Person in Charge: D. H. Stork

Scientific and Professional Staff: H.-U. Bengtsson, C. D. Buchanan, D. A. Park, and W. E. Slater

Scope of Work

The primary activity of this experimental group is to study e^+e^- annihilations at the highest energy storage ring (PEP at SLAC) available in the U.S. Data are gathered with the Time Projection Chamber facility (PEP-4) which recently completed a successful year of data taking (77 inverse picobarns). The UCLA group built and put into operation two photon calorimeters that cover the 10 percent of solid angle at the polar regions of the detector. Participation in the PEP-4 experimental program occurs at several levels in addition to production of this hardware. They are actively engaged in (a) physics analysis, particularly two-photon annihilation reactions, (b) in writing analysis programs for the detector, and (c) in doing Monte Carlo calculations (one of them being Deputy Spokesman). Since two detectors (PEP-4 and PEP-9) share the interaction region (IR2), an extended collaboration has developed to study two-photon reactions.

In a second activity at the Split Field Magnet facility at the ISR at CERN, one of staff members studied high transverse momentum proton-proton collisions which yield information about the scattering and fragmentation of quarks and gluons. Study of the fragmentation process in terms of QCD color strings provides a natural connection between the p-p activity and the e^+e^- work at PEP.

Goals and/or Major Results to Date

A partial list of topics on which results have been obtained from the first running cycle of the TPC includes: Searches for fractionally charged particles, charged hadron production, prompt electron and muon production, proton-, lambda-, neutral K meson-, Gamma-, neutral Pi meson-, Phi- and K*- production, and particle correlations. A major effort at extracting results from combined PEP-4 and PEP-9 data has begun to be productive on several topics: Untagged gamma-gamma to two and four charged particles, and eta and eta-prime meson production are examples.

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UNIVERSITY OF CALIFORNIA
Los Angeles, California

Title of Project: Research in High Energy Physics (Theoretical)

Person in Charge: N. Byers

Scientific and Professional Staff: N. Byers and two graduate student research assistants, V. Zambetkis and J. Malenfant; formerly G. Adkins and R. McClary

Scope of Work

Research is in relativistic quantum field theory and theoretical elementary particle physics with particular application to bound states. The group studies relativistic and radiative effects in onium spectroscopy; positronium and quarkonium. Research is also conducted on electroweak interaction theory; radiative corrections to $\nu_\mu e$ scattering have been calculated, also neutrinoless double beta decay in connection with the possibility of nonvanishing neutrino mass, and spontaneous symmetry breaking due to a two doublet Higgs sector.

Goals and Major Results to Date

Electroweak Interactions. Radiative corrections to $\nu_\mu e$ scattering appropriate for the present generation of bubble chamber experiments were calculated (with R. Ruckl and A. Yano). Order α radiative corrections to both ortho and para-positronium were recalculated, a discrepancy removed, and a gauge consistent method of calculating these corrections to all orders was found. Strong Interactions. Inclusion of $(v/c)^2$ relativistic and radiative corrections to E1 radiative decay widths in charmonium was found to remove an existing discrepancy between nonrelativistic theory and experiment. Such effects were calculated using the Cornell model potential for E1 and M1 rates in both the charmonium and Υ system. In addition, vacuum polarization-coupled channel effects were found to be appreciable.

Goals are now to study and calculate vacuum polarization-coupled channel effects using better models for the confining forces than have been used to date. In addition, work is going on in the electroweak theory to obtain predictions from the two Higgs doublet model of spontaneous symmetry breaking at SSC energies. Also, relativistic and radiative corrections to the one photon decay of mu-muonium are under study and will be computed in the program of studying the behavior of the wave function at the origin for a relativistic bound state.

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Title of Project: Study of Hadronic Interactions with Polarized Beam and Targets in the 0.5-12 GeV/c Range

Person in Charge: G. Igo

Scientific and Professional Staff: G. Igo, G. Pauletts, C. Newsom, and A. Wang

UNIVERSITY OF CALIFORNIA
Los Angeles, California

Scope of Work

The group's current primary activity is the study of polarization phenomena in the kaon-nucleon interaction. Current experiments include kaon elastic and inelastic scattering from deuterons in the 1.5 GeV/c range. They also are studying pion-nucleon polarization phenomena. The experiments are done at the National Laboratory for High Energy Physics (KEK) in Tsukuba, Japan.

Goals and/or Major Results to Date

The goal is to do enough experiments to uniquely determine (within reasonable experimental uncertainties) the kaon-nucleon amplitude in the region above the first inelastic thresholds (K-n and K-Δ) and extending up to the limits imposed by the KEK proton synchrotron (about 2.0 GeV/c). This is the region where Z^* resonances have been proposed by other groups working in this energy region. Initial results have been obtained for the asymmetry in π-$\vec{d}$ elastic scattering at 0.76 GeV/c and are being prepared for publication. Measurement of the asymmetry in K-$\vec{d}$ elastic scattering at 1.5 and 1.7 GeV/c are being analyzed.

A further experiment is planned at KEK to measure the spin rotation angle, β, in K^+-p elastic scattering, thus determining a triad of experimental quantities ($d\sigma/dt$, A_y, and β) sufficient to determine the scattering amplitude. In addition, large P_T measurements in the reaction $\vec{p} + \vec{d}(\vec{n})$ are planned when the polarized beams at KEK are available (1985).

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Title of Project: High Energy Physics Phenomenology

Person in Charge: A. Soni

Scientific and Professional Staff: None

Scope of Work

The purpose of this program is to conduct research in the theory and phenomenology of elementary particle physics. In particular, the phenomenological implications of quantum chromodynamics (QCD) and electroweak models will be pursued with the aim of providing an important link between theory and experiment.

In the area of QCD the theory and phenomenology of the new type of bound states of QCD called glueballs is being vigorously investigated. This work should then provide suggestions to experimentalists for searching these new types of particles and furthermore it should provide tests for experimental candidates.

UNIVERSITY OF CALIFORNIA
Los Angeles, California

In the area of electroweak theories and weak decay of new heavy quarks (such as charm, bottom, and top), the reported anomalies in W,Z decays, the CP violation parameter ϵ', and other hints for potential deviations from the standard model will be examined. This should then provide clues for a new electroweak theory beyond the standard model.

Goals and/or Major Results to Date

The bound state spectrum of glueballs and the interactions of low lying glueballs with quarks, gluons, and hadrons has been investigated. The widths for the decays of low lying scalar and pseudoscalar glueballs to photons and to vector mesons have been calculated and some interesting sum rules were derived.

The effects of the so-called annihilation graph for b-quark decays has been examined. The implications of the recently measured b-lifetime for various important parameters of the standard model were calculated and the constraints provided by them for a variety of interesting phenomena were investigated.

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UNIVERSITY OF CALIFORNIA
Los Angeles, California

Award No.: DE-AT03-83ER40120

Title of Project: Experimental, Theoretical, and Computational Studies of the Plasma Beat Wave Accelerator

Persons in Charge: C. Joshi and F. F. Chen

Scientific and Professional Staff: J. M. Dawson, C. E. Clayton, and T. Katsouleas

Scope of Work

This group is studying a new collective accelerator concept called the Plasma Beat Wave Accelerator which has the potential of producing acceleration gradients in excess of 1 GeV/m. Acceleration is achieved by space-charge waves in a plasma propagating with velocities close to c driven by resonantly beating two laser beams. On the experimental front, the scope of work is on producing and diagnosing homogenous plamas, generating and diagnosing the plasma wave, and checking the growth and saturation characteristics of the longitudinal electric field. On the theoretical and computational, fronts they are studying the questions of phase-locking the particles in the plasma wave, laser beam depletion, beam-loading, and growth of emittance.

Goals and/or Major Results to Date

During FY 1983 this group made signficiant advances in:

1. Producing a homogeneous plasma source and detecting a plasma wave produced by beating two counter propagating beams by transverse Thomson Scattering: B. Amini and F. F. Chen, Phys. Rev. Lett., to be published.

2. Two dimensional computer simulations of the Plasma Wave: (work done in conjunction with the Los Alamos Group): C. Joshi, et. al., Nature, to be published.

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UNIVERSITY OF CALIFORNIA
Riverside, California

Award No.: DE-AT03-76ER70107

Title of Project: Collider Physics

Person in Charge: A. Kernan

Scientific and Professional Staff: W. Guryn, K. Morgan, D. Pitman, and D. Smith

Scope of Work

This group is studying proton-antiproton interactions at center-of-mass energy 540 GeV. The experiment (UA1) is conducted at the CERN SPS Collider by an international collaboration of approximately 130 scientists. The collaboration has constructed a general purpose hermetic detector with neutrino detection capability. The aim of the experiment is the study of the interactions of the point-like constituents--quarks and gluons--of the nucleon. The study of quark-antiquark interactions, in particular, allows a test of the electroweak model of Glashow, Weinberg, and Salam.

During the construction phase (1978-1981), this task built a luminosity monitor consisting of eight high precision drift chambers for measuring proton-antiproton elastic scattering. They also provided two 3-meter long drift chambers for the forward arms of the detector. Subsequently they developed a strong data analysis activity at U.C. Riverside based on a VAX 11/780 computer and a MEGATEK 3-dimensional graphic system.

Goals and/or Major Results to Date

The experiment has met its stated goals of finding the W and Z bosons and the high transverse momentum jets of the Standard Model. The present aims are to search for the predicted sixth quark, to measure the W and Z parameters more accurately, and to look for phenomena beyond the Standard Model. These goals necessitate an upgrade of the detector calorimetry and the addition of a microvertex detector. The latter device is currently under construction by this task. In parallel with the detector upgrade, an increase in luminosity from the present 10^{29} cm^{-2} sec^{-1} value to close to 10^{31} cm^{-2} sec^{-1} is anticipated over the next few years.

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Title of Project: SLAC Experiment

Person in Charge: B. C. Shen

Scientific and Professional Staff: W. Gorn, J. G. Layter, B. C. Shen, and G. J. VanDalen

UNIVERSITY OF CALIFORNIA
Riverside, California

Scope of Work

The primary activity of this group is the experimental study of e^+e^- interactions at high energies, utilizing the unique capabilities of the PEP-4 TPC detector facility at SLAC. This collaboration of LBL, UCLA, UCR, Johns Hopkins, Massachusetts, Tokyo, and Yale is currently carrying out a systematic analysis of both one photon annihilation and two photon scattering at PEP, studying 80 pb^{-1} of data at 29 GeV CM energy.

The group has designed and constructed the inner and outer drift chambers which serve as trigger elements for the Time Projection Chamber. Scheduled running will incorporate the 15 Kg superconducting solenoid to improve momentum resolution and gating grids on the TPC to suppress background and reduce track distortion, enabling the detector to operate at its full capability.

The group will continue to pursue the study of fundamental interaction in e^+e^- physics at high energy storage ring facilities.

Goals and/or Major Results to Date

The PEP-4 TPC collaboration has contributed the following new results: improved limits on the production of charge 1/3, 2/3, and 4/3 particles; the most complete measurements of inclusive particle cross sections; the first detailed study of baryon production; studies of resonance production; heavy quark fragmentation; the study of flavor correlations in multihadron production; the first examination of $\pi\pi KK$ final states produced in two-photon interactions.

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UNIVERSITY OF CALIFORNIA, SAN DIEGO
La Jolla, California

Award No.: DE-AT03-81ER40028

Title of Project: Studies of Elementary Particles (Experimental)

Person in Charge: O. Piccioni

Scientific and Professional Staff: W. Mehlhop, C. Enscoe, and P. Bowles

Scope of Work:

The group studies the results of picture data obtained during an experiment at BNL with apparatus built at the UCSD campus. The measurements of the pictures were also done with measuring projectors built by the group. The processing of the digital data is done utilizing the computer on campus. The subject of the research is the fundamental elementary particles and their interactions.

A line distinguishable from the above, but still based on the study of elementary particles and their interactions, is the study of the Einstein-Podolsky-Rosen (EPR) paradox, both theoretically and experimentally.

Goals and/or Major Results to Date

Several years ago they conceived of a new method to study high energy interactions. The method appeared applicable to an important section of interactions, namely those called with the vague name of "diffractive." Essentially, the method consisted in taking data of events when the collision with a nucleus produced secondary mesons and also produced the excitation of a given level in the target nucleus. One could then isolate types of interactions which occurred with the transmission of a quantum compatible with that particular nuclear transition.

The interest in that goal was first and mainly in the demonstration that the method could be used. Secondly, they hoped to contribute to the study of resonance, particularly to the much debated A1 resonance.

The goal of demonstrating the feasibility of the method is achieved. They also have shown the remarkably low cross section to produce the "nondiffractive level" 15.1 MeV in carbon, both for scattering and for three meson production, and are very close to finishing the analysis for the diffractive level 4.4 MeV in carbon and for three meson production.

For the EPR they have devoted much effort to provoking as many discussions as possible with outstanding theorists on the ground basis of the EPR. They have produced a presentation of the argument in a way which is not found in the literature, concluding that either there exists in nature a miraculous action at distance or the EPR phenomenon is not acceptable according to current quantum mechanics. In the numerous debates, they have always reached the point where the debater quit the discussion having no reply to their presentation. They thus maintain that the "general opinion" is without an acceptable defense.

Their presentation also avoids any reference to Bell's relations which, though a beautiful work, have obscured the real point of the EPR for years. They have written a paper which will appear in the book "Open Questions in Quantum Mechanics" edited by van der Merwe and Tarozzi (publisher: Reidel). At the same time, being convinced that the EPR needs a solution and not a snobbish brush off, they are working at studying the correlation of the planes of polarizations of the photons from the annihilation of positrons. They have put together a complex apparatus of a novel type and have been taking data for a few months.

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UNIVERSITY OF CALIFORNIA
San Diego, California

Award No.: AT03-81ER40029

Title of Project: Theoretical High Energy Physics

Persons in Charge: N. Kroll, J. Kuti

Scientific and Professional Staff: S. Gottlieb, N. Kroll, J. Kuti, A. Longhitano, A. Patel, D. Toussaint, D. Wong

Scope of Work

The research supported by this program is devoted to the investigation of theoretical elementary particle physics. Recent investigations include studies of lattice field theory models, lattice quantum chromodynamics, electroweak processes, cosmology, the interaction of slow magnetic monopoles with matter, electromagneitc instabilities in free electron lasers, and the theory of laser driven accelerators. A major portion of our current effort is devoted to the development and implementation of computational methods in lattice field theories. These efforts are being supported by a special purpose Ising processor and an ST-100 Array Processor with Cray-1 computing power.

Goals and/or Major Results to Date

In the area of lattice field theory models the critical properties of the 3d-Ising model were determined to very high accuracy by a special purpose Ising processor, and Monte Carlo studies of spinless fermions with short range interactions in 2+1 dimensions were carried out successfully. Furthermore a novel stochastic method was developed and elaborated for the calculation of the eigenvalues and wave functions of lattice quantum Hamiltonians and Transfer matrices.

In lattice Quantum Chromodynamics the meson-meson and baryon-meson couplings of strong interactions were calculated using Monte Carlo techniques. The critical point of thermal quark liberation in lattice QCD was investigated very accurately and the approach to scaling was studied in detail. The renormalization group beta function of lattice QCD was determined from gluon thermodynamics.

The theory of the interaction of slow monopoles with matter was further developed. A general conclusion which emerges is that the utility of doped helium proportional counters for detection of slow monopoles is confirmed, and that in addicion to being more calculable, there is some likelihood that they are better for this application than other noble gas counters.

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UNIVERSITY OF CALIFORNIA, SANTA BARBARA
Santa Barbara, California

Award No.: DE-AT03-76ER70023

Title of Project: Elementary Particle User Group at Santa Barbara

Persons in Charge: D.O. Caldwell, R.J. Morrison, and M.S. Witherell

Scientific and Professional Staff: R. Eisberg, P. Karchin, A. Lu, S. McHugh, and S. Yellin

Scope of Work

At SLAC, a part of the group has been involved in a two-photon annihilation experiment, PEP-9. Data have been taken and more will be taken next year, but because of problems with PEP-4, which serves as the central detector, the current year is being spent analyzing data. This is the only experiment at PEP or PETRA designed specifically to study processes involving the collision of two high energy photons.

At Fermilab, the tagged photon beam originated by UCSB, has been used with a multiparticle spectrometer to study charm photoproduction. The analysis of E-516 has been completed, and a Tevatron experiment, E-691, is now being prepared by another part of the group. The main new addition to the spectrometer is a silicon microstrip detector, which is being built by UCSB.

In conjunction with members of the Instrumentation Group at Lawrence Berkeley Laboratory, a large experiment is being prepared to search for neutrinoless double beta decay, in order to test lepton number conservation and look for effects of neutrino mass and right-handed currents. The apparatus utilizes 1.4 liters of Ge (8 detectors) inside a NaI active shield.

Recently the group has become involved in designing the SLD apparatus for the SLAC Linear Collider. Work has been done on both the liquid Argon system and the Cerenkov ring imaging detector.

Goals and/or Major Results to Date

The PEP-9 analysis so far has concentrated on double-tag and single-tag data, with some work in collaboration with PEP-4 on no-tag. Results have been obtained on the electromagnetic structure function of the photon, the total γ-γ cross section, and the Q^2 (mass of one virtual photon) dependence of the η,η',f_0,f_0^1, and A_2 mesons, as well as of the mysterious 4π ($\rho\rho$) bump around 2 GeV. The E-516 results include measuring the branching ratios, $\frac{D^0 \to K^-\pi^+\pi^0}{D^0 K^-\pi^+}$, and the $D^0 \to K^-\rho^+$ branching fraction, which are relevant to the D decay mechanism. The measured Υ inelastic photoproduction cross section agrees with QCD but not muon experiments. The details of D^* photoproduction have also been obtained.

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UNIVERSITY OF CALIFORNIA
Santa Barbara, California

Award No.: DE-AT03-84ER40136

Title of Project: Electron Acceleration by Laser Fields in a Gas

Person in Charge: J. R. Fontana

Scientific and Professional Staff: J. R. Fontana and D. Rentschler

Scope of Work

Microwave linacs used for high-energy electron acceleration have inherent limitations both in acceleration gradient and bunch charge due to the effect of the walls. High-power pulsed lasers can provide large fields, coherent over a considerable volume, by means of focusing surfaces located far enough to operate at low power density, thus avoiding damage. In this project, a particular laser acceleration mechanism is studied which uses a gas in the interaction region to match the phase velocity of the laser fields to the electron velocity, and so obtain cumulative interaction. At high particle energies, collision effects are small, and the principal limitation involves the maximum laser field allowed by the onset of gas breakdown phenomena.

Goals and/or Major Results to Date

A comparative analysis has been made of electron passes through laser beams of different configurations, using normalized variables for generality. For the same laser power, Gaussian beam modes give smaller interaction than a cone of plane waves incident at the Cherenkov angle, meaning that the latter configuration is advantageous for practical applications, although it is not a spherical mirror resonator mode. The effect of collisions between electrons and gas molecules is analyzed by a distribution function method. A partial differential equation describes the evolution in phase space of the properties of an electron bunch moving through the gas while interacting with the laser field.

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UNIVERSITY OF CALIFORNIA, SANTA CRUZ
Santa Cruz, California

Award No.: DE-AT03-76ER70197

Title of Project: Electronic Detectors/e^+e^- Physics

Persons in Charge: D. Dorfan, C. Heusch, and A. Seiden

Scientific and Professional Staff: R. Hamilton, L. Kopke, W. Lockman, R. Partridge, J. Perrier, H. Sadrozinski, T. Schalk, and A. Weinstein

Scope of Work

The Santa Cruz experimental group is presently involved in two major efforts: the MARK III detector at the SPEAR Storage Ring at SLAC and the MARK II upgrade for first experimentation at the SLAC Linear Collider. The goal of the MARK III is the study of mesons produced in the decay of the J/Ψ, the study of weak decays of the D^0 and D^+, and the measurement of the mass, production cross section, and decay channels for the F, Λ_c, Σ_c, Σ_c^*. To produce these particles they use the annihilation of e^+e^- in the 3 to 5 GeV energy range at SPEAR. They are simultaneously working on the MARK II upgrade whose goals are the detailed study of the Z^0 intermediate vector boson at the SLAC Linear Collider using the annihilation of e^+e^- beams in the 100 GeV energy range. Physics topics presently foreseen are: measurement of the Z^0 mass and width, tests of the Standard Model through the coupling of quarks and leptons to the Z^0, search for t-quarks, search for the Higgs meson, QCD tests via multi-jet studies, and determination of the number of light neutrinos. The group has also maintained a strong interest in detector technology with special emphasis on drift chambers and calorimetry.

Goals and/or Major Results to Date

The principal goals on the MARK III have been to accumulate approximately an order of magnitude more data than presently exists on the physics topics described above. To date, results presented have been mainly on J/Ψ decays, which have included a first determination of the spin and parity of the η_c and evidence for a new narrow state at 2.2 GeV in radiative decays.

In addition they have accumulated a substantial amount of D decay data and expect first results in the summer of 1984.

Most of the MARK II upgrade construction is expected to be completed in the next year and initial data taken on the Z^0 in 1987.

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UNIVERSITY OF CALIFORNIA
Santa Cruz, California

Title of Project: Research in High Energy Physics

Person in Charge: A. Litke

Scientific and Professional Staff: D. Gelphman, R. Lee, and A. Litke

Scope of Work

This group is doing research in experimental high energy physics, with an emphasis on experiments performed at electron-positron colliding beam machines. They have three projects under way. First, they are studying the charmonium system made from a charm quark and an anti-charm quark. This work is based on data taken with the Crystal Ball detector at the SPEAR e^+e^- storage ring at SLAC. The Crystal Ball consists of a spherical array of NaI crystals and is able to detect photons above 10 MeV over a large solid angle with excellent energy resolution. Second, they are investigating radiative transitions in the bottomium system consisting of a bottom quark and an anti-bottom quark. The data for these studies are being taken at the DORIS e^+e^- ring at DESY, again with the Crystal Ball detector. Third, they are part of the Mark II detector collaboration for the experimental program at the SLAC Linear Collider. The major goal of this program is the detailed study of the Z^0 intermediate vector boson. The initial contribution (in collaboration with a group from the University of Hawaii) is the development of silicon micro-strip detectors for possible use as a secondary vertex detector in the Mark II.

Goals and/or Major Results to Date

The work on charmonium includes measurements of some of the fundamental properties of the $^3P_0$ and $^3P_2$ charmonium states. Also, they have found a large and perplexing suppression of the radiative decay $\psi' \to \gamma\eta$ compared to $J/\psi \to \gamma\eta$.

The study of bottomium has yielded measurements of the three radiative transitions $\Upsilon' \to \gamma\chi_b$. They have presented evidence for a narrow state ζ with a mass of 8.3 GeV/c^2 observed in radiative Υ decays. They are now taking additional data in order to confirm (or deny) the existence of this unexpected state.

The Z^0 physics program at the SLC is expected to begin in 1987.

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CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California

Award No.: DE-AC03-81ER40050

Title of Project: Nonaccelerator Physics

Person in Charge: B. Barish

Scientific and Professional Staff: B. Barish, J. Elliott, C. Lane, and G. Liu

Scope of Work

Two nonaccelerator projects are under way:

One research effort is devoted to developing detectors for GUT monopoles. In particular, different noninductive techniques are being investigated. A prototype acoustic device to detect the thermoacoustic pulse from eddy current losses in a conductor has been built. In addition, a scintillator array detecting monopoles by time of flight is presently taking data.

A second effort is on the DUMAND project. DUMAND is dedicated to deep underwater detection of muons and neutrinos. The Caltech group has responsibility for the instrumentation module, where acoustic sensors will be used to place and monitor the position of the array.

Goals and/or Major Results to Date

The monopole project is aimed at determining a design for a very large scale detector array. Such questions as whether the experiment can be done at sea level or needs to be underground, types and redundancy of detectors, etc. are being addressed.

The immediate goal for DUMAND is to develop and deploy a short prototype string (6 phototubes). This device will prove the ability to collect and transmit data to shore, measure backgrounds, and detect muons and upward going neutrinos. If this step is successful, they anticipate building a large array for studies of high energy neutrino interactions.

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Title of Project: Phenomenology

Person in Charge: G. C. Fox

Scientific and Professional Staff: G. C. Fox, F. Fucito, W. Furmanski, T. Gottschalk, M. Johnson, S. Otto, A. Patel, and P. Stolorz

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Pasadena, California

Scope of Work

The phenomenology group pursues research at the interface of theoretical and experimental high energy physics and some areas of computer science. There are three main fields of research.

The major thrust of the group is the exploration of the predictions of theory (Quantum Chromodynamics - QCD) for a variety of important processes such as e^+e^- annihilation and hadron-hadron scattering. In particular, they are interested in the difficult problems concerned with modeling hadron final states. Another activity is the field of lattice gauge theories where their research covers both numerical work and development of new techniques such as the use of improved actions. The third major field involves the development and use of new computer architectures to tackle large scale high energy physics calculations. This activity is part of an interdisciplinary research program at Caltech which involves the construction and use of concurrent processors in a broad range of science and engineering fields.

Goals and/or Major Results to Date

The goals include development of realistic models for hadronic final states which include known theoretical and phenomenological constraints. They have made significant progress in this regard although they still need further research especially in the area of gluon fragmentation.

The numerical program in lattice gauge theories is built around new algorithms and construction of new hardware of increased performance. They recently completed the first reasonably large (64 element) concurrent processor which can be applied to a wide range of problems. This machine has equivalent performance to 8 VAX11/780's and is now being used to investigate quantum field theories numerically.

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Title of Project: Theory

Person in Charge: Murray Gell-Mann

Scientific and Professional Staff: L. Castellani, R. Feynman, S. Frautschi, F. Fucito, M. Gell-Mann, M. Gunaydin, B. Morel, J. Patera, D. Politzer, J. Preskill, A. Sagnotti, J. Schwarz, S. Solomon, N. Warner, M. Wise, and F. Zachariasen

Scope of Work

The work of the theory group focuses on the following major areas: supergravity as a potential description of quantum gravity and of the unification of all particle interactions; supersymmetry as a theoretical laboratory and as a possible phenomenological description of high energy physics grand unified theories; application of unified theories to astrophysics and cosmology (axions, monopoles, baryon generation inflation, and the like), studies in perturbative QCD at high energies and nonperturbative QCD at low energies (both by lattice methods and by consideration of nonlinear Dyson's equations); and the phenomenology of the "standard model" of strong and electroweak interactions.

Goals and/or Major Results to Date

1. Forge a unification of all particle interactions with the aid of supergravity ideas (e.g., the superstring theory of Green and Schwarz, which gives N=8 supergravity in the appropriate limit) together with the evolving data;

2. Understand the early universe in terms of particle theory (e.g., the Preskill, Wilczek, and Wise theory of galaxy formation based on axions and the Abbott and Wise predictions of anisotropy of the observable microwave background);

3. Expand the predictive power of the established low energy theories: QCD and the electroweak model.

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Title of Project: Mark III at SPEAR

Person in Charge: D. Hitlin

Scientific and Professional Staff: D. Coffman, G. Dubois, J. Hauser, D. Hitlin, J. Richman, and R. Schindler

Scope of Work

The Mark III is a general purpose detector optimized for the reconstruction of exclusive final states in e^+e^- annihilation in the SPEAR energy region (3 to 7 GeV/c^2). It has been operational since spring 1982. Data has to date been taken at the ψ and ψ resonances emphasizing radiative decays of the ψ and weak decays of D mesons produced at the ψ. Future running is planned to study F mesons, charmed baryons, and τ leptons. The interest in discoveries at the ψ may also warrant additional data taking in that region.

Goals and/or Major Results to Date

The Mark III has, in its ψ sample of 2.7 million events, found evidence for the ξ (2220), a surprisingly narrow resonance which decays to KK; has measured the spin-parity of the η_c for the first time; has found the $\gamma\rho$ decay mode of the iota; and has found evidence for a complex structure most likely composed of several new resonances in $\gamma\rho\rho$ and $\gamma\eta\pi\pi$ final states. Analysis of these results, emphasizing the search for evidence for glueball or hybrid states, is continuing.

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The ψ'' sample has yielded precise new measurements of the ratio of D^0 and $D^\pm$ lifetimes, the discovery of several new Cabibbo-allowed and Cabbibbo-suppressed D hadronic decay modes, and a substantially improved limit on $D^0\bar{D}^0$ mixing. Continued analysis of the D sample will provide a more complete understanding of the mechanism of weak decay of charmed particles. Future data will be aimed at increasing this understanding by confronting models with new information of the decay of F mesons and charmed baryons.

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Title of Project: SLD at SLC

Person in Charge: D. Hitlin

Scientific and Professional Staff: D. Hitlin, C. Mathews, R. Schindler, and Y. Zhu

Scope of Work

The SLD is a new detector intended for the study of final states in e^+e^- annihilation at Z^0 energies produced at the new SLAC Linear Collider. This detector is fully competitive with the new generation of detectors at LEP. It incorporates a high precision CCD vertex detector, a 100 μm resolution drift chamber, Cerenkov ring imaging devices and high quality electromagnetic and hadronic calorimetry. The calorimeter is divided into a uranium-liquid argon section (LAC) three absorption lengths deep, placed inside the 1 Tesla superconducting solenoid and an additional five absorption lengths using gas readout tubes embedded in the magnet flux return steel.

The SLD will study the physics of Z^0 decays, with particular emphasis on determination of standard model parameters, jet studies, and searches for new phenomena, such as Higgs or supersymmetric particles. The expected completion date is 1988.

Goals and/or Major Results to Date

The development of the uranium-liquid Argon calorimeter is the particular responsibility of the Caltech group. A successful mechanical prototype has been constructed, which has demonstrated the feasibility of achieving highly segmented projective tower geometry in an all metal (uranium plus stainless steel) structure. Development of electronics for the readout and digitization of the ionization chamber pulses is under way. A beam test of a section of the LAC, incorporating the actual mechanical design and readout electronics is planned for the coming year.

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Pasadena, California

Title of Project: Search for Nucleon Decay

Person in Charge: J. LoSecco

Scientific and Professional Staff: G. Blewitt, B. Cortez, and J. LoSecco

Scope of Work

They are involved in a test of grand unified theories of elementary particle interactions using the 8000 ton IMB detector in Cleveland, Ohio. In particular, they are looking for evidence for the decay of the proton or bound neutron. Such a process is forbidden by all known interactions and would be indicative of new, previously unknown physics, at a very high energy scale. The detector is quite flexible and in addition to the search for nucleon decay, they are also exploring atmospheric neutrino interactions, searching for magnetic monopoles, looking for neutron-antineutron oscillations sensitive to the burst of neutrinos from a supernova explosion in our galaxy and setting limits on neutrino oscillations.

The device, an imaging water Cherenkov counter, is unique. It has a high sensitivity to the processes in question yet is capable of background rejection to the level of less than one background event per year for some decay modes.

Goals and/or Major Results to Date

They have operated this detector for well over a year. Over half of the data recorded has been fully analyzed. They have failed to find evidence for the decay $p \to e^+\pi^0$ and set a lower bound on the lifetime for this mode of 2×10^{32} years. This is more than an order of magnitude longer than theoretical expectations. In addition, they have results on about 12 other decay modes, magnetic monopoles, and neutron-antineutron oscillations.

Work is continuing. In particular, they are very concerned with increasing the detector resolution by improvements in hardware and software. They are also deeply involved in trying to quantify the impact of the neutrino background on the various physics objectives.

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Title of Project: MARK J Experiment

Person in Charge: H. Newman

Scientific and Professional Staff: S. Braunstein, R. Mount, H. Newman, H. Stone, and R. Y. Zhu

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Pasadena, California

Scope of Work

The MARK J experiment is continuing its study of e^+e^- interactions at the PETRA storage ring at DESY in Hamburg, West Germnay, up to 46 GeV center-of-mass energy. The detector is optimized for the clean identification and momentum measurement of muons and for calorimetric measurements of energy flow.

The Caltech group has played a leading role in the development of the software for data analysis and Monte Carlo simulations. The recent emphasis of the group has been in jet analysis and tests of QCD. Some of this work has been carried out in cooperation with the phenomenology group.

Coordination of the software task has involved the development of an international computer network, which has also served as the pilot project for a larger network required for the LEP3 experiment.

Goals and/or Major Results to Date

Measurement of the muon pair charge asymmetry with a systematic error of < 1 percent confirming the Glashow-Weinberg-Salam electroweak theory; discovery of three jet events in e^+e^- annihilation; experimental tests of OCD by measuring the rate of production and the shape of three and four jet events, and by energy-energy correlations; measurement of R from $\sqrt{s}$ = 12 to 46 GeV; search for the top quark, for new heavy leptons, for supersymmetric scalar partners of the nuon and tau, for excited muon and electron states, for charged Higgs, technipions, and for other new particles; measurement of the semileptonic branching ratios, fragmentation functions, and charge asymmetries of charm and bottom quarks, QED determined valid down to 10^{-16} cm; confirmed the point-like nature of the known leptons and quarks to 10^{-16} cm; determination of the weak neutral current coupling constants in purely leptonic interactions.

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Title of Project: LEP3 Experiment

Person in Charge: H. Newman

Scientific and Professional Staff: S. Braunstein, F. Carminati, R. Gomez, R. Mount, H. Newman, H. Stone, and R. Y. Zhu

Scope of Work

The LEP3 experiment is based on a 6 meter radius magnetic detector which is optimized for the precision measurement of photons, electrons, muons, and hadronic jets. The experiment is being performed by more than 500 physicists from 33 institutions in 13 countries, including 13 U.S. universities.

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Pasadena, California

The Caltech group has the overall responsibility for the development of the computing systems for off-line data analysis, for an international computer network needed to coordinate the daily activities of the collaboration, and for the development of the software base in cooperation with a team of experts based at CERN.

The Caltech group is also responsible for the development of calibration techniques for controlling the relative gains of the 12,000 bismuth germanate crystals comprising the electromagnetic calorimeter to < 1 percent. This will be a determining factor in achieving the necessary resolution for inclusive photon and Higgs missing mass measurements.

They have begun the in depth investigation of the mechanism responsible for the sensitivity of BGO light output to radiation damage in the crystals, of detecting the trace impurities responsible, and of reducing the radiation damage effect. This work is being carried out in cooperation with several research groups at Caltech in the physics, chemistry, and geology departments, and at the reactor at UC Irvine.

Goals and/or Major Results to Date

The special features of the LEP3 detector are uniquely suited for precise measurements in the framework of the standard electroweak theory and for the search for scalar particles such as the Higgs by missing mass measurements of the type of $e^+e^- \to \ell^+\ell^- + X(\ell = e,\mu)$. The high resolution measurements of lepton and jet energies and angles give them maximum sensitivity for detecting a variety of new, unexpected phenomena.

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Title of Project: Crystal Ball Experiment

Persons in Charge: C. W. Peck and F. C. Porter

Scientific and Professional Staff: C. Edwards, R. Partridge, C. Peck, F. Porter, and P. Ratoff

Scope of Work

The Crystal Ball experiment is currently taking data on the decays of the Υ resonances at the DORIS e^+e^- storage ring at DESY, in Hamburg, West Germany. The principal thrust of the effort is to examine the radiative decays of these particles as a tool in the study of the strong interaction. Much of this work is directed toward the discovery and measurement of new particles containig a b and an anti-b quark. In addition, the decays of the $\Upsilon(1S)$ resonance are being analyzed to search for possible gluonic effects and for more exotic possibilities, such as particles predicted in supersymmetric theories.

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Prior to the move to DORIS, the Crystal Ball experiment was used to take a large sample of data on the charmonium system at SPEAR (SLAC). There are still several interesting topics to be examined in these data, and analysis of the SPEAR data thus continues to be an ongoing and exciting endeavor.

The Caltech group in the Crystal Ball collaboration has continuing responsibility for the monitoring and maintenance of the photomultiplier measurement of the light from the NaI. The Caltech group has also had major responsibilities from the beginning in the software design and maintenance. In addition, the Caltech component is very active in the physics analysis of the data and has made substantial contributions to most of the major results from the experiment.

Goals and/or Major Results to Date

The Crystal Ball collaboration has begun to produce results from the analysis of data taken at DORIS. Recently, the existence of at least two χ_b states was confirmed by the Crystal Ball. With the more recent addition of new data, they hope to measure the properties of these states as well as find additional states.

In the analysis of the SPEAR data, several important results have been obtained by the Crystal Ball experiment, including the discovery of the η_c and η_c' charmonium pseudoscalar states and of the θ and other interesting effects in the J/ψ radiative decays which might have something to do with "gluonic" mesons. Work continues, especially on the latter topic, and additional results will be forthcoming from the analysis of these data.

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Title of Project: DELCO at PEP

Persons in Charge: B. Barish and R. Stroynowski

Scientific and Professional Staff: B. Barish, D. E. Koop, F. B. Mills, L. Z. Rivkin, W. Ruckstuhl, M. Sakuda, S. S. Sherman, R. Stroynowski, and H. Yamamoto

Scope of Work

The group is studying the electron-positron annihilations at high energies. The experiment is performed in collaboration with SLAC Group A (Prescott, Atwood) and Stanford/SLAC Group G (Wojcicki, Kirkby). Its main emphasis is on the studies of the properties of heavy quarks and tau leptons. The detector is optimized for excellent particle identification and is particularly well suited for the study of direct electrons. The Caltech group is actively participating in every aspect of the experiment, including construction, data taking, calibration, and data analysis.

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Pasadena, California

Goals and/or Major Results to Date

Study of the direct electrons produced in e^+e^- annihilations resulted in excellent measurements of the semileptonic branching ratios of the charmed and bottom quarks and in determination of their fragmentation functions. Other studies of the c and b quarks are still being pursued with the goal of measuring the lifetimes of particles containing these quarks. Good particle identificiation allowed for the measurements of the Cabibbo suppressed tau lepton decays and for stringent tests of the standard model of electroweak interactions.

The LEP3 detector, with its large magnetic volume, is also readily adaptable for e^+e^- studies up to 180 GeV, and $p\bar{p}$ studies to 10 TeV in the center of mass during later phases of LEP. The LEP3 detector has good mass resolution up to the 1 TeV mass scale for a muon pair.

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Title of Project: Mark II/SLC

Persons in Charge: B. Barish, C. Peck, and R. Stroynowski

Scientific and Professional Staff: B. Barish, G. Fox, T. Gottschalk, M. Nelson, C. Peck, E. Sonderstrom, and R. Stroynowski

Scope of Work

The experiment uses the Mark II detector to study the physics of the intermediate vector boson Z^0 at SLC. The upgraded detector is sufficiently powerful and general to measure the mass and width of Z^0 and to determine the number of light neutrinos. It will allow for the tests of the standard model of electroweak interactions and for the search for the top quark and Higgs particles. As the first experiment in the relatively clean e^+e^- annihilation environment at these energies, it will also search for new, unexpected phenomena.

Goals and/or Major Results to Date

At present, the group is actively participating in the upgrade of the detector by constructing the time-of-flight counters, designing the drift chamber calibration system, and developing track finding programs for the new drift chamber. Substantial involvement in data taking, physics analysis, and phenomenology of the results is also planned.

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CARNEGIE-MELLON UNIVERSITY
Pittsburgh, Pensylvania

Award No.: DE-AC02-76ER03066

Title of Project: Counter Spark Chamber Group

Person in Charge: R. M. Edelstein

Scientific and Professional Staff: R. M. Edelstein, J. S. Russ, R. J. Lipton, D. Potter, and C. Forsyth

Scope of Work

In two Fermilab experiments, the group has been working on the measurement of hadronic production of heavy quark states. The first involved a prompt muon trigger and a passive target in a two-arm spectrometer using an all electronic detector system and a run using a triggerable optical system viewing a NaI scintillating live target. Data were also taken in this experiment on high P_T direct photons and π^0 produced in a 300 GeV proton beam.

The second experiment uses a hybrid emulsion spectrometer to measure lifetimes for charm and bottom states produced by 1 TeV protons in an upcoming first stage Tevatron experiment. The group is providing the liquid argon electromagnetic calorimeter for this project.

Advanced detector development is a new effort for the group. Currently, interest centers on work on an optical system to view scintillations in capillary tubes filled with liquid scintillant, avalanche chambers, and Cerenkov ring imaging detector devices.

Goals and/or Major Results to Date

In the earlier experiment, a signal has been seen of unlike sign μe pairs produced in a 200 GeV π^- beam, signifying charm production at the 20 μ barn cross section level. Also, a substantial data set has now been culled from the proton run of the experiment of high P_T direct photons and π^0's produced in association with charged particle jets. Results will soon be available for the γ/π^0 ratio out to $P_T < 6$ GeV and for γ/hadron-jet correlations.

In the forthcoming hybrid emulsion experiment lifetimes of $D^\pm, D^0, F, \Lambda_c$, etc. will be measured with high precision for several thousand charm events, and lifetimes for B states will be measured for ~200 events. Charm and bottom decay modes and production dynamics will also be measured.

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CARNEGIE-MELLON UNIVERSITY
Pittsburgh, Pennsylvania

Title of Project: X-ray Group

Persons in Charge: R. B. Sutton

Scientific and Professional Staff: R. B. Sutton

Scope of Work

1. This group, in collaboration with groups from other universities, has pursued a program of measurement of particle properties through observation of the x-rays from exotic ($\bar{p}$, Σ^-, K^-) atoms. The latest work has involved measurement of the Σ^- magnetic moment. No work beyond this fiscal year is planned in this field.

2. In collaboration with the group of A. Engler, et al, work is proceeding toward the construction of BGO crystal arrays for the luminosity monitor and small angle tagger for LEP-3. This involves investigation of properties of BGO such as radiation damage, energy, and spatial resolution of arrays of crystals for high energy electrons in the SLAC test beam and use as a detector of small angle events at the PEP-9 intersection region.

Goals and/or Major Results to Date

1. The Σ^- magnetic moment has been measured to be $1.11\pm.031\pm.011$ nuclear magnetons.

2. New information on the effects of radiation on BGO has been obtained. The spatial and energy resolution for assemblies of BGO crystals for high energy (~10 GeV) electrons has been obtained. The use of BGO crystal assemblies as a tagger for small angle events at e^+e^- intersection regions has been studied; the observation of Bhabha scattering events at PEP-9 has been made.

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Title of Project: Theory Group

Person in Charge: R. E. Cutkosky

Scientific and Professional Staff: R. E. Cutkosky, M. J. Levine, L.-F. Li, L. Wolfenstein (on sabbatical leave, 1983-1984), E. Remiddi (Visitor academic year 1983-1984), C. Maxwell, and P. Pal

Scope of Work

The Theory Group pursues basic theoretical physics research in the main areas of high energy physics: the phenomenology of weak interactions, including grand-unified models; quantum electrodynamics, including analytical and numerical calculations; strong interactions, including phenomenology and the basic properties of QCD.

In addition, members of the group frequently consult with experimental colleagues on goals and results of experiments and assist in organizing common facilities and in organizing formal and informal seminars. Contributions are made to the pedagogical as well as to the scientific literature, and to workshops and conferences in the form of reviews and summaries as well as in presentation of original research.

Goals and/or Major Results to Date

Members of the Theory Group are engaged in, and have produced important results in the following research topics: the phonomenology of CP violation, neutrino masses, baryon decay, and Higgs particles; the confinement problem in QCD and the formulation of perturbative and nonperturbative methods, and also hadron phenomenology; numerical and computer-based algebraic and analytical calculations of high order graphs in QED, including the development and use of a powerful highly-parallel computer.

These topics are directed toward crucial questions concerning our understanding of the structure of matter, and also assist in the development of methods of general utility.

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Title of Project: Colliding Beams Group

Persons in Charge: A. Engler

Scientific and Professional Staff: A. Engler, R. W. Kraemer, H. Vogel, I. Brock, G. J. Bobbink, and C. Rippich

Scope of Work

1. The members of this group are working at the DORIS II Storage Ring at DESY, Hamburg, West Germany. They are using the Crystal Ball detector in collaboration with groups from the United States and Europe. This experiment started data taking in 1982 and has recently completed the first part of its program. During the current year, further data are expected. A new research proposal has recently been submitted to the DESY directorate using the same detector.

2. They are also part of the LEP3 collaboration. This effort is directed toward the construction of a very large detector to be used at the LEP Storage Ring at CERN. This new machine is expected to begin operation at the beginning of 1989. The responsibilities involve radiation tests of BGO and design and construction of a luminosity monitor and two photon taggers.

Goals and/or Major Results to Date

The main purpose of the Crystal Ball experiment is to study radiative transitions in the upsilon system. During the past year, they have observed three photon lines in the decay of the Υ' (2S) meson. These correspond to the transitions $2^3S_1 \rightarrow 1^3P_{0,1,2}$. The splitting between these P-states is a measure of the spin orbit coupling in the $b\bar{b}$ interaction.

The main goal in the LEP3 experiment is a study of electroweak phenomena. They are particularly interested in the properties of the Z^0 and a search for the Higgs scalar meson.

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UNIVERSITY OF CHICAGO
Chicago, Illinois

Award No.: DE-AC02-80ER10587

Title of Project: Theoretical Studies of High Energy Phenomena

Person in Charge: R. G. Sachs

Scientific and Professional Staff: R. G. Sachs

Scope of Work:

Basic theoretical physics of high energy phenomena, especially those bearing on CP and T violation and on the structure of hadrons. Interpretation of high energy experiments in consultation with experimenters. Hands-on training of graduate students in phenomenological theory by participation in research.

Goals and/or Major Results to Date

Goals include the identification of theoretical and experimental methods for understanding the origins of CP and T violation and the elucidation of the phenomenological analysis of the structure of hadrons. Results that have been obtained concern (1) origins of CP violation at the level of the six quark model, (2) the information concerning the structure of baryons obtained from measured magnetic moments, and (3) the corresponding information concerning the structure of constituent quarks, i.e., their anomalous moments.

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Title of Project: Measurement of the Decay Parameters in Polarized $\Sigma^- \to n e \bar{\nu}$ with High Precision

Person in Charge: R. G. Sachs and R. Winston

Scientific and Professional Staff: D. Muller, E. C. Swallow, R. Winston, H. Hsueh, and G. Zapalac

Scope of Work

This group's primary interest is the weak interactions of hadrons. Specifically, they have been performing experiments on the beta decays of hyperons which test the structure of the semi-leptonic interaction of quarks with leptons. In a recently completed experiment at Fermilab (Charged Hyperon Collaboration E-715), they measured the beta decays of polarized Σ^- hyperons. The matrix element for this process is predicted to be effectively "V+A" by the Cabibbo SU(3) model. However, previous experiments with polarized Σ^- have persistently failed to confirm this distinctive prediction of the theory. Their experiment is the first high statistics (~100,000 polarized beta decays) test of this critical issue.

UNIVERSITY OF CHICAGO
Chicago, Illinois

Goals and or Major Results to Date

In the recently completed Fermilab experiment E-715 approximately 10^5 beta decays from a Σ^- beam (up to 20 percent_polarization) were detected. The electron asymmetry from polarized $\Sigma^- \to ne\nu$, and in particular its sign, is a distinctive prediction of the Cabibbo model. They have now analyzed $\approx 1/3$ of the data for the electron asymmetry and reported its value at the DPF Santa Fe Meeting in November. Since their apparatus permits a complete kinematic reconstruction of each decay, they will ultimately determine all the form-factors from their data. In addition, the Σ^- magnetic moment will be determined with greater precision than from past measurements with $\Sigma^- \to n\pi^-$ because the analyzing power of the beta decays is much greater than that of the non-leptonic decays.

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UNIVERSITY OF CHICAGO
Chicago, Illinois

Award No.: DE-AC02-82ER40073

Title of Project: Elementary Particle Theory

Person in Charge: J. L. Rosner

Scientific and Professional Staff: J. D. Bjorken, L. Brekke, I. Duniets, D. Hochberg, A. Kagan, Y. Kitazawa, D. London, C. Quigg, J. Rabin, J. Rosner, K. Tesima, and A. Trivedi

Scope of Work; Goals and/or Major Results to Date

Topics studied include soluble models of QCD (Bjorken and Trivedi), composite fermions and Higgs bosons (Brekke), branching ratios in nucleon decay (Duniets), polarized electron-proton scattering and lattice gauge theories (Hochberg), supersymmetric particle detection (Kagan), radiative corrections to Z and W decay (Kitazawa), magnetic monopoles (London and Rosner), prospects for future physics at a very large collider (Quigg), definitions of integration over supersymmetric variables (Rabin), production and detection of massive neutral leptons and new heavy gauge bosons (Rosner), multiparticle production (Tesima). The focus is diverse as befits the many directions in which progress in particle theory is taking place.

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UNIVERSITY OF CHICAGO
Chicago, Illinois

Award No.: DE-AC02-80ER10773

Title of Project: Particle Physics and Cosmology

Person in Charge: M. S. Turner

Scientific and Professional Staff: A. Melott, D. N. Schramm, M. S. Turner, F. Accetta, J. Frieman, and R. Scherrer

Scope of Work

This group pursues basic theoretical research at the interface between particle physics and cosmology/astrophysics. Members of this group interact with and/or collaborate with other astrophysicists and physicists at Chicago, Fermilab (theoretical and theoretical astrophysicists group), and physicists at other universities (e.g., Penn, Bartol, Harvard, ITP/UCSB). The work of the group is twofold. First, the early universe (with its essentially unlimited energy budget and high particle fluxes) and various contemporary astrophysical sites (e.g., neutron stars, red giant stars) with their unique physical environments are used as "nontraditional" high energy physics laboratories, providing windows to physics at energies ($\gg 10^3$ GeV) and regions of phase space (e.g., particle masses and couplings) which are not accessible in terrestrial laboratories. Second, modern particle theory (e.g., the SU(3) X SU(2) XU(1) model, grand unified theories, supersymmetric/supergravity models, etc.) are applied to the early universe, in an attempt to unravel the detailed early history of the universe (SSB phase transitions, baryogenesis, quark/hadron transition, primordial nucleosynthesis, and galaxy formation).

Goals and/or Major Results to Date

Projects completed during the past year include: analysis of the origin and evolution of density perturbations in the new inflationary Universe scenario, establishment of very stringent bounds on the flux of relic monopoles based upon various astrophysical arguments, use of primordial nucleosynthesis to obtain bounds on the number of light neutrino species (≤ 4) and the baryon-to-photon ratio, and the study of galaxy formation in the presence of exotic (e.g. relic particles from "the bang") dark matter.

Current projects include: continued study of inflationary models, of galaxy formation in model universes dominated by exotic relics; continued use of primordial nucleosynthesis to constrain particle properties; study of the propagation and origin of ultra high energy cosmic rays; analysis of the effect(s) of light, Nambu-Goldstone bosons on stellar evolution (as a possibility for inferring the existence of such particles by astrophysical observations).

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UNIVERSITY OF CINCINNATI
Cincinnati, Ohio

Award No.: DE-FG02-84ER40153

Title of Project: Inelastic Strong Interactions at High Energies

Person in Charge: P. Suranyi

Scientific and Professional Staff: F. Mansouri and J. Scanio

Scope of Work

The group has been engaged in various aspects of theoretical high energy physics. Present investigations are focused in two general areas. The first is a study of lattice gauge theories. Various methods of calculation have been and are being examined in an attempt to understand first the structure of Abelian models and then the structure of non-Abelian models. Both analytic methods and numerical methods are expected to yield important information concerning the nature of these theories.

Studies of theories of gravity and their relationship to particle physics are also in progress. These theories are being looked upon from the point of view of a gauge theory, an approach which is indispensable in the construction of unified theories including gravity. Investigations of higher dimensional space-times are under way and the conformal symmetries of such spaces are being studied in detail.

Goals and/or Major Results to Date

Various methods giving increasingly more precise, but physically equivalent, results were introduced for the investigation of Abelian lattice theories. Various parameters of the theories were estimated in Hamiltonian lattice theories by employing variational methods and by constructing periodic Gaussian models.

A systematic method for performing dimensional reduction on theories constructed in higher dimensional space-times was developed. For various cases the equations of motion were completely worked out. An extended conformal theory of gravity was constructed and extensions to superspace were also studied.

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CLARKSON UNIVERSITY
Potsdam, New York

Award No.: DE-FG02-84ER40144

Title of Project: Application of Nonlinear Dynamics to the Beam-Beam Interaction

Person In Charge: T. C. Bountis

Scientific and Professional Staff: M. Bier and V. Papageorghiou

Scope of Work

In recent years, the principles and methods of Nonlinear Dynamics have been successfully applied to the problem of the beam-beam interaction in colliding beams of high energy accelerators. With the aid of these methods the important phenomena of resonances, sensitive dependence on initial conditions, beam blow-up, etc. can be studied numerically and analytically even in regimes of high nonlinearities (or strong beam-beam force).

Using the techniques of Nonlinear Dynamics they have so far: (a) studied by iterative and perturbative methods and periodic solutions and their stability of a differential equation of two beams interacting in one space dimension, (b) analyzed a 4-dimensional model of difference equations describing two colliding proton (antiproton) "round" beams, with equal, and unequal, x and y "tunes" Ω^1, Ω_2, (c) developed an Action-Angle variable approach for the regions of attraction of resonances in colliding electron beams, and (d) studied numerically certain restabilization and orbit transport properties of area-preserving maps, which have potential applications to the proton beam-beam interaction problem.

The main objectives of the work proposed here are: (a) to study, using techniques of Nonlinear Dynamics, the combined effects of dissipation and quantum fluctuations in electron (positron) colliding beams, (b) to investigate in detail the effect of synchrotron oscillations in "bunched" beams, and (c) to extend all earlier results to colliding beams with "eliptically" symmetric charge distributions.

Goals and/or Major Results to Date

Major results to date include: (a) the analytical and numerical determination of the regions of stable solutions of linear and non-linear Hill's equations describing the beam-beam interaction in "flat" beams, (b) a resonance analysis of colliding "round" p, $\overline{p}$ beams with equal and unequal "tunes" Ω_1, Ω_2 which has enabled them to find regions of $\sigma = \Omega_2/\Omega_1$ values over which blow-up effects are minimized, (c) the extension of this analysis to e^+, e^- "round" beams (including radiation damping) and the approximate determination of regions of attraction of particle orbits, and (d) the study of bifurcation properties of periodic orbits and escape rates of orbits in area-preserving mapping models of colliding beams.

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UNIVERSITY OF COLORADO
Boulder, Colorado

Award No.: DE-AC02-81ER40025

Title of Project: Experiment E516, 691 and SLD

Person in Charge: U. Nauenberg

Scientific and Professional Staff: J. Elliott, L. Cremaldi, G. Schultz, and D. Edmonds

Scope of Work

This group has pursued over the last five years a study of the dynamics of photoproduction of hadronic states in hydrogen. These experiments have covered the photon energy range up to 150 GeV and hadronic state masses of 10 GeV. This study will continue during the Tevatron era where they will have photons up to 250 GeV and masses up to ~ 14 GeV. The efforts have been to study charm photoproduction; single particle ($\pi K^0, \Lambda^0$) spectra and high p_t spectra. They are trying to determine whether they observe jet like structure in these processes.

The future goal, years hence, is to study Z^0 decays with the SLD detector. In that vein they have begun to help with the R&D necessary to build the detector.

Goals and/or Major Results to Date

They have recently obtained results on the study of charm photoproduction and J/ψ photoproduction on protons. These show that the charm quark is quite hard and the hadronization shows the charm meson carrying approximately 60 percent of the incident protons energy. These results are very similar to those in e^+e^-. They are finalizing their work on single particle spectra and their implication on what model applies to describe hadronic photoproduction.

Their goal is to determine a good model for the photoproduction of hadronic final states.

For the future they want to search for the Higgs, determine the number of neutrinos, and study phenomena associated with Z^0 decays using the SLD detector.

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Title of Project: Theoretical Physics

Person in Charge: T. A. DeGrand

Scientific and Professional Staff: K. T. Mahanthappa, D. R. T. Jones, and F. Graziani

UNIVERSITY OF COLORADO
Boulder, Colorado

Scope of Work

This task funds theoretical research in particle physics at Colorado (except for T. DeGrand). The members of the group primarily study the electroweak interactions and grand unification, with some work on quantum chromodynamics and some work on lattice field theory. Work on grand unification encompasses phase transitions in the early universe and supersymmetry. Studies on supersymmetry have included some model building (also involving supergravity), investigations of the beta function in model supersymmetric field theories, and work on the supersymmetric standard model of grand unification. Work on quantum chromodynamics involves studying the gluon condensate and its effects on charmonium sum rules. In lattice field theory they are investigating alternative Monte Carlo methods for gauge theories.

Goals and/or Major Results to Date

They have recently shown how to compute the two-loop beta function in a supersymmetric gauge theory from a one-loop calculation, using the anomaly. A supersymmetric grand unified theory based on SU(5) with no light super partners and no fine tuning was constructed. A novel Monte Carlo approach to Hamiltonian gauge theories measured string tensions and (for the first time) string widths in lattice U(1) gauge theory.

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Title of Project: Outstanding Junior Investigator Program

Person in Charge: T. A. DeGrand

Scientific and Professional Staff: T. A. DeGrand

Scope of Work

Task C is funding through the Outstanding Junior Investigator Program. for a theoretical physicist interested, at present, in problems in strongly interacting systems such as the candidate theory for the strong interactions, quantum chromodynamics. Much of the work involves inventing or carrying out numerical studies of these systems. Specific problems to which contributions are made include: the role of topological excitations in confinement, the behavior of QCD at high temperature (above the deconfinement transition), both with and without quark, and studies of one-dimensional fermion systems.

Recently work was also done on the phenomenology of baryon polarization in inclusive hadron production at high energy and small momentum transfer.

UNIVERSITY OF COLORADO
Boulder, Colorado

Goals and/or Major Results to Date

Last summer C. DeTar of Utah and T. DeGrand gave a fairly convincing argument that the confinement-deconfinement phase transition in QCD at high temperature, which is known to be first order when only gluons, with no

quarks, present, is smoothed out like a liquid-gas transition above the critical point if quark masses are sufficiently small.

Recently, the most accurate Monte Carlo simulation of a fermion system performed to date was completed, in studying a one-dimensional field theory of interest to condensed matter physics--a lattice version of the Gross-Neveu model. They studied the behavior of solitons as a function of fermion coupling and proved the existence of soliton doping: i.e., adding fermions to a half-filled band leads to spontaneous creation of solitons.

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Title of Project: Colorado Group on E-400 and E-687 at Fermilab

Person in Charge: J. P. Cumalat

Scientific and Professional Staff: P. Coteus, D. Edmonds, and G. Schultz

Scope of Work

This group is studying the production of heavy flavors in photoproduction (E-687) and hadroproduction (E-400).

Of primary interest in hadroproduction is to measure the charm cross section on different nuclei as a function of energy.

In photoproduction, the ψ and Υ cross sections will be measured and the level of "Beauty" production will be determined.

Goals and/or Major Results to Date

E-400 is in the midst of data taking. The data at 400 GeV has been accumulated and soon the experiment will resume data taking at 800 GeV.

The immediate goal for E-687 is to finish building the beam line and experiment for running in early 1986.

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Title of Project: Electron-Positron Physics with MAC and Mark II

Person in Charge: W. T. Ford

Scientific and Professional Staff: E. Fernandez and J.G. Smith

UNIVERSITY OF COLORADO
Boulder, Colorado

Scope of Work

This group is engaged in the study of fundamental processes, particularly electroweak interactions, induced by electron-positron annihilation at high energies. Colorado's part in the development of the MAC detector included construction of the central tracking chamber and associated software. The physics emphasis so far has been on testing the standard model of electroweak forces as manifested in muon and tau lepton pair production, universality of the weak interactions among the elementary fermion families (lifetime of the tau lepton and of the bottom-flavored hadons), and searches for the new particles predicted by supersymmetry theories. As part of the Mark II/SLC collaboration, the group is now embarked on a program to extend these studies to processes occurring at energies around the Z^0 resonance.

Goals and/or Major Results to Date

Major results include the first detection of the relatively long lifetime of the bottom-flavored hadrons, a high-precision measurement of the electroweak charge asymmetry in muon pair production, and an upper limit on the mass of a possible supersymmetric partner of the electron.

Primary goals include a measurement of the number of fermion families, search for Higgs scalars, and study of properties of the Z^0.

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COLUMBIA UNIVERSITY
New York, New York

Award No.: DE-AC02-76ER02271

Title of Project: Theoretical High Energy Physics

Person in Charge: T. D. Lee

Scientific and Professional Staff: N. H. Christ, E. D'Hoker, G. Feinberg, R. Friedberg, O. Martin, A. H. Mueller, P. Nason, A. E. Terrano, E. J. Weinberg, and T. D. Lee

Scope of Work

The major activity is in various fundamental aspects of field theory and high energy physics. Interest extends from the quantization of gravity, applications of QCD, lattice gauge theory, to supersymmetry and cosmology.

In order properly to take into account the effect of fermion loops in QCD, this group is pioneering the development of parallel processors for lattice QCD.

For the purpose of eliminating divergence difficulties in quantum gravity, a new discrete mechanics has been developed; in place of the usual continuum theory they deal only with systems of finite degrees of freedom per unit volume, yet retain all the symmetry properties of the usual theory (Poincare invariance, Lorentz symmetry, unitary symmetry, and the general invariance of Einstein's coordinate transformations) plus the unitarity of the S-matrix.

Goals and or Major Results to Date

At present this group has just completed the 16-node parallel processor, which should have the equivalent computing capability of a dedicated CRAY-1. Over the next year they hope to finish the 256-node, and that would enable one, for the first time, to include fermion loops in QCD for a 20x20x20x40 lattice.

They have extended the usual perturbative QCD to include various "non-perturbative" corrections, such as renormalons and multiplicity distributions in gluon and quark jets. They hope eventually to calculate with accuracy all asymptotic predictions of QCD. Investigation of the monopole solutions in gauge theory has led to an active interest in cosmology. They expect this investigation to continue in the years to come.

The discrete mechanics that they have developed have already been successfully applied to classical mechanics, non-relativistic quantum mechanics, relativistic field theories including QCD, and more recently to general relativity. In all these cases it is found that systems with finite degrees of freedom can be constructed which retain the full symmetry of the corresponding continuum theories. They are beginning to investigate the quantum effect of gravity and hope to derive new and interesting results.

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UNIVERSITY OF CONNECTICUT
Storrs, Connecticut

Award No.: DE-AC02-79ER10336

Title of Project: Investigations in Particle and Field Theory

Persons in Charge: K. Haller and M. M. Islam

Scientific and Professional Staff: D. Caldi, K. Haller, M. M. Islam, and P. Mannheim

Scope of Work

Research is being performed in basic theoretical physics relevant to current problems in particle and field theory, including the following: Gauge theory (lattice and continuum studies), grand unified models, hadron structure and dynamics, theoretical analysis of high energy $\bar{p}p$ and pp scattering, solitons and topological objects, mechanisms of spontaneous and dynamical symmetry breaking, theory of proton decay, Majorana neutrinos and Grassmann spin.

Members of the group participate in conferences, workshops, summer institutes, collaborate in research at central high energy physics facilities, and present seminars and colloquia on their work to other particle physics groups. Visitors to the group discuss their work with them and a vigorous in-house seminar program maintains scientific contacts within the group.

Goals and/or Major Results to Date

Members of the group have produced results on the following topics: Grand unified theories consistent with failure to observe positron decay mode of the proton; canonical quantization of classical Grassmann spin; Monte Carlo calculations in 3-D SU(2) lattice gauge theory, leading to graphic evidence for flux tubes; quantum theory of the pure gauge spectrum of non-Abelian gauge fields, and its relation to color confinement; work on sigma model and soliton theory; dynamics of soft CP violation as a by-product of a spontaneously broken gauge symmetry; predictions of $\bar{p}p$ and pp elastic differential cross sections at Tevatron energy based on a valence quark model of the nucleon.

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CORNELL UNIVERSITY
Ithaca, New York

Award No.: DE-AC02-83ER40089

Title of Project: Simulation of Ultra-Low Emittance Electron Storage Rings

Person in Charge: L. N. Hand

Scientific and Professional Staff: None

Scope of Work

The work involves computer simulation of both existing and possible types of electron accelerators. It is intended to model as closely as possible the various physical effects which would determine the normalized emittance in real machines. Initial work will be concentrated on effects which affect the emittance at very low intensities. If time permits, intensity dependent effects (wake fields, intrabeam scattering, etc.) will be examined in detail. The emphasis will be on locating areas where technological improvement will be necessary in order to build real machines.

Goals and/or Major Results to Date

This project is a computer simulation of an electron storage ring which, due to ultralow beam emittance, could serve as either a source of coherent x-rays or as a model for the damping ring at a high energy linear collider.

For the latter purpose $\epsilon\gamma/N$ must be minimized (ϵ is the transverse beam emittance, γ the Lorentz contraction factor and N the number of particles being accelerated). The design goal* for $\epsilon\gamma/N$ is about 30 times less* than is presently being achieved at the SLC project at Stanford.

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CORNELL UNIVERSITY
Ithaca, New York

Award No.: DE-AC02-80ER10569

Title of Project: Collective Acceleration of Ions Using High Current Realistic Electron Beams

Persons in Charge: J. A. Nation, C. E. Seyler, and D. Sullivan

Scientific and Professional Staff: A. Anselmo, M. Arman, M. Campbell, D. Fenstermacher, S. Greenwald, J. Ivers, G. Kerslick, J. Nation, and C. Seyler

Scope of Work

Participants in this program are pursuing theoretical and experimental studies of various schemes for the accelerators of ions in a slow space charge wave supported on a weakly relativistic electron beam.

Analytic theory and numerical simulation techniques are employed to study nonlinear wave propagation on electron beams in inhomogeneous waveguides. Two codes are employed, one a fluid M.H.D. code, and the other a particle in cell simulation.

The experimental effort utilizes the electron beam pulse power facilities at Cornell to generate a 1.0 kA, 200 + 450 KeV electron beam. Space charge waves are grown on the beam which are then studied as the waves travel through an inhomogeneous guide. Experiments are in progress to study ion acceleration in the space charge waves. The wave phase velocity is externally controlled.

Goals and/or Major Results to Date

Experimental control of wave phase velocity in a converging guide has been demonstrated. Electric field strengths at the beam location of greater than 20 MV/m have been obtained. These results compare well with the fluid simulation code results which have shown stable soliton like wavetrains propagating with fields of greater than 10 MV/m. A demonstration proton accelerator using a beatwave generated by propagation of a space charge wave through a rippled magnetic field has been carried out. The M.R.C. particle-in-cell simulations have been used to model wave growth on the electron beam.

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UNIVERSITY OF DELAWARE/FRANKLIN INSTITUTE
Newark, Delaware

Award No.: DE-AC02-78ER05007

Title of Project: Particle Theory, Cosmology, and Relativity

Persons in Charge: T. K. Gaisser and G. Steigman

Scientific and Professional Staff: T. K. Gaisser, Q. Shafi, and G. Steigman

Scope of Work

The members of this group are engaged in basic research in elementary particle theory and related areas of cosmology, astrophysics, and cosmic rays. Their emphasis is on interdisciplinary aspects of particle physics; the strategy is to use insights and information from related fields to make progress in particle theory and vice versa. Being a small group, they collaborate extensively with physicists at other institutions, both theorists and experimentalists. Topics under active study currently include grand unified theories, monopoles, inflationary universe, neutrino physics with nucleon decay detectors, properties of interactions at ultra-high energies, primordial nucleosynthesis, and massive neutrinos (and other inos) in astrophysics and cosmology.

Goals and/or Major Results to Date

Recently a systematic calculation has been made of the cosmic ray neutrino flux at the various nucleon decay detectors. This can be used for background calculations, for intercalibration of detectors and as the basis of a search for neutrino oscillations. A detailed comparison of the predictions of primordial nucleosynthesis with the observed abundances of the light elements has led to restrictive upper and lower bounds to the nucleon density as well as a significant constraint to the number of species of light neutrinos. Cosmological bounds to the mass of neutrinos or other inos have been derived from the observed large scale structure and evolution of the universe. A simple prescription for successfully implementing the inflationary scenario in the context of grand unified theories (GUTS) has recently been presented. The properties of monopoles that appear in GUTS larger than SU(5) and in Kaluza-Klein (K-K) theories have been elaborated. It has been shown that if GUTS are embedded in K-K theories, significant modifications of the standard GUT predictions for proton decay and $\sin^2\theta_W$ are to be expected.

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DUKE UNIVERSITY
Durham, North Carolina

Award No.: DE-AS05-76ER03065

Title of Project: Experimental Elementary Particle Physics

Person in Charge: W. D. Walker

Scientific and Professional Staff: L. Fortney, A. T. Goshaw, W. Kowald, and W. J. Robertson

Scope of Work

The major projects that this group has been involved in over the last four years have been:

1. A measurement of the lifetime of charmed mesons.
2. The properties of the ρ' meson (a radial excitation of the ρ).
3. A study of meson production in hadron-nucleus collisions.
4. A search for glueballs and other boson resonances.
5. Technical work on bubble chambers.

The group was previously involved in experimental work using visual techniques, a bubble chamber being the main element in the experiments. They are now involved in three experiments which are totally electronic, two at FNAL and one at BNL.

Goals and/or Major Results to Date

The main results of the last several years have had to do with the measurement of the lifetimes of the D^0 and $D^\pm$ mesons. Measurements indicate a lifetime of the D^0 which is nearly an order of magnitude greater than what was the accepted value when the experiment was started. They are continuing this work with even better resolution using the small CERN chamber, LEBC. They should be able to investigate the properties of the Λ_c and possibly the F meson.

A by-product of the charm experiment has been the study of a resonance which is probably a radial excitation of the ρ meson. This experiment allows a far more detailed study of the properties of the ρ' than has previously been possible. The radiative widths of other resonances will also be measured.

They are studying the subject of $\overline{p}$ annihilation in complex nuclei using data from FNAL experiment E597. This is part of a general program designed to study the multi-pion production in hadron-nucleus collisions.

Future Goals

They are newly involved in three major experiments which promise to give very interesting physics results. They are in a consortium which

DUKE UNIVERSITY
Durham, North Carolina

proposes to seek evidence for the existence of a quark-gluon plasma. In such an environment, quarks would become deconfined for a short period of time. This phenomena would show itself by means of a phase transition in the quark matter. This experiment will be done in the C0 straight section of the Fermilab $\overline{p}p$ collider. They are also involved in a Fermilab experiment designed to study charm (and possibly beauty) meson production using 1000 GeV protons from TeV II. A run at Fermilab should produce data on χ mesons within the next year.

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UNIVERSITY OF FLORIDA
Gainesville, Florida

Award No.: DE-AS05-81ER40008

Title of Project: High Energy Theory

Persons in Charge: R. D. Field, P. Ramond, and C. Thorn

Scientific and Professional Staff: T. L. Curtright, M. Doria, R. D. Field, R. Holman, P. Ramond, P. Sikivie, and C. Thorn

Scope of Work

Participants in this program pursue basic physics research in various areas of high energy theory and phenomenology. The program covers a broad range of subjects such as quantum field theory, quantum chromodynamics, grand unified theories, and the interface between particle physics and cosmology. There is an active visitor and seminar program which brings to Gainesville prominent physicists to share their research results and expertise with this group. In addition, members of the group travel and participate in many national and international physics conferences and workshops.

Goals and/or Major Results to Date

During the 1983-1984 academic year, the members of the Particle Theory Group have been very productive, publishing over 20 papers and producing important results on such topics as: Liouville quantum field theory, axions, B-L violation in supersymmetric SU(5), conformally invariant field theories, baryon production in e^+e^- annihilations, standard model constraints on fermions, the direct photon spectrum in the inclusive decay of the upsilon, etc.

It is the intention of the group to continue to actively participate in the further development of high energy physics. The research performed by this group involves crucial questions at the forefront of our understanding of the structure of matter.

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FLORIDA STATE UNIVERSITY
Tallahassee, Florida

Award No.: DE-AS05-76ER03509

Title of Project: Experimental High Energy Physics

Person in Charge: J. E. Lannutti

Scientific and Professional Staff: J. Albright, J. H. Goldman, S. Hagopian, V. Hagopian, J. Lannutti, D. Levinthal, F. Lopez, and B. Pifer

Scope of Work

The group's primary work is the study of hadronic resonances and hadronic interactions using counters, chambers, and electronic techniques. At present, the group is analyzing data from three major experiments that utilized multiparticle spectrometers. In the two experiments run at Fermilab, hadronic resonances that had $K_S^0K_S^0$, $K^0\Lambda$, $\Lambda\bar{\Lambda}$ and $\phi\phi$ in the final states are under study. A third experiment was performed at BNL using the multiparticle spectrometer to study the charateristics of the E decaying into $K^+K^0\pi^-$. In an extension of this BNL experiment, an order of magnitude more data will be gathered utilizing a time-of-flight counter to identify the K^+.

A new research thrust currently under way is the study of multiparticle correlations, jet production and high-p_T one- and two-particle correlations at the Tevatron. These studies are in two distinct experiments, one using the MPS and the other a stand-alone experiment for which they are building the needed drift chambers. For this latter experiment, they have the primary responsibility for all aspects of the data. Both of these Tevatron experiments will be run in 1984 and early 1985.

The conversion from the bubble chamber techniques to counter techniques for experiments is now completed. This group has taken major responsibility for data reduction and analysis in all of the above experiments.

Goals and/or Major Results to Date

The $K_S^0K_S^0$ data sample produced charmed D's decaying into K^*K^0. The other final states observed, including $\Lambda\bar{\Lambda}$, have enabled evaluations of cross sections for some standard resonances at 200 GeV. The $\phi\phi$ experiment has seen abundant production of ϕ's and $K^*(890)$'s at 400 GeV/c. The BNL MPS experiments have produced five cascade resonances, the best lower limit of baryonium production in exchange type reactions and copious production of E mesons. The current goal is to understand the E by a spin parity analysis and to determine the spin 0 content in the E mass region (the location of a strong candidate for a "glueball").

The goal of the Tevatron experiments is to study both low and high multiplicity events, especially at high transverse momentum. The non-MPS

FLORIDA STATE UNIVERSITY
Tallahassee, Florida

experiment should produce data at extremely high transverse momentum (up to 15 GeV/c).

Further experiments are planned at TeV I and using $\overline{p}p$ and the D^0 detector. Some members are also working on projects related to SSC, the planned 20 TeV pp collider.

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Title of Project: Theoretical High Energy Physics

Person in Charge: J. E. Lannutti

Scientific and Professional Staff: A. Devoto, P. A. M. Dirac, D. W. Duke, L. Halpern, J. D. Kimel, C. J. Maxwell, and J. F. Owens

Scope of Work

The theory group has two distinct areas of interest--high energy physics (Devoto, Duke, Kimel, Maxwell, Owens) and gravitational theory (Dirac, Halpern).

In the area of high energy physics, the efforts have been focused most strongly on applications of perturbative quantum chromodynamics to processes involving large momentum transfers. Topics studied include large transverse momentum jet, hadron, and photon production; deep inelastic lepton-hadron scattering phenomenology; heavy quark hadron and photoproduction; and the study of the photon structure functions. In addition, members of the theory group routinely work with experimentalists offering assistance in the interpretation of new results as well as in the planning of new experiments.

The gravitational program has been involved with calculations aimed at testing various consequences of Dirac's "large number hypothesis."

Goals and/or Major Results to Date

Completed calculations include next-to-leading-order calculations for the photon structure function, deep inelastic Compton scattering, and the nucleon longitudinal structure function. Extensive work has also been done on the phenomenology of deep inelastic lepton-hadron scattering including the determination of simple parametrizations for the parton distributions in the nucleon. Numerous results concerning large transverse momentum jet, hadron, and photon production have also been published.

The gravitational group has been involved in analyses of data obtained from lunar missions and the Martian landers in an effort to test Dirac's predictions concerning the time dependence of the gravitational coupling. An investigation of some new solutions of Einstein's general relativistic field equation is also under way.

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UNIVERSITY OF GEORGIA
Athens, Georgia

Award No.: DE-FG09-84ER40160

Title of Project: High Energy Hadron-Hadron Collisions

Person in Charge: T. T. Chou

Scientific and Professional Staff: T. T. Chou

Scope of Work

The effort is focused on the phenomenological study of log s physics in hadron collisions. Experiments performed at Fermilab, CERN ISR, and SPS Collider have been analyzed and interpreted with the geometrical model, which emphasizes the diffraction aspects and associated phenomena in high energy hadron-hadron scattering. Some specific predictions based on this model have been proposed which can be compared with future experiments. The present main activities are concentrated on elastic scattering and diffractive dissociation at ultra-high energies, the multiplicity distribution, forward-backward correlations and other related phenomena in particle production processes, and high energy hadron-nucleus collisions.

Goals and/or Major Results to Date

The geometrical model has been quite successful in the comparison of its predictions with experiments up to ISR energies. These include the existence and the shift of the positions of the first dip and the second maximum with increasing energy, and the rise of the second maximum, in pp, $\bar{p}p$ and np scattering, the prediction of meson radii, the existence of dips in πp and Kp elastic processes, and π-nucleus diffractive dissociation. At the Collider energy, the elastic scattering model remains valid, and recent analysis of inelastic collision data suggests that the forward-backward charge distribution is binomial and the observed large multiplicity fluctuation is mainly due to the fluctuation of the impact parameter.

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GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, Georgia

Award No.: DE-AS05-81ER40003

Title of Project: Dissipative Effects in the Beam-Beam Interaction of Intersecting Storage Rings

Persons in Charge: J. Ford and F. Vivaldi

Scientific and Professional Staff: None

Scope of Work

This group is investigating various dynamical instabilities which arise in high energy intersecting storage rings due to the beam-beam interaction. The particle dynamics are simulated by means of three degrees of freedom models, which are studied with various analytical and numerical methods of nonlinear mechanics. The object of this research is to obtain conditions for global beam stability over long time scales, as a function of the machine parameters. The efforts are focused on the study of the so-called "weak instabilities", which are processes peculiar to systems with more than two degrees of freedom. This class of phenomena constitutes the ultimate limit to the beam stability.

Goals and/or Major Results to Date

The most recent major result has been the derivation of an analytical expression for the coefficient of modulational diffusion, the weak instability induced by synchrotron oscillations. The analysis is applicable to a large class of conservative beam-beam models.

The present goal is to extend these results to the case of dissipative systems.

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HARVARD UNIVERSITY
Cambridge, Massachusetts

Award No.: DE-FG02-84ER40158

Title of Project: The Theory of High Energy Collision Processes

Person in Charge: T. T. Wu

Scientific and Professional Staff: C. L. Schultz and C. Iredale

Scope of Work

Strong interactions at high energies have the following properties: 1) relativistic kinematics, 2) particle production, 3) unitarity, and 4) isospin invariance. On the basis of relativistic quantum field theories with or without isotopic spin, they have obtained a simple physical picture, called the impact picture, which gives a number of unusual predictions, including for example, the increasing total cross section and the rising plateau. Many of these predictions have been verified experimentally. With the recent operation of the CERN $\bar{p}p$ Collider, verifications have become possible at the much higher center-of-mass energy of 540 GeV. First results at this Collider from the UA1 and the UA4 Collaborations are in excellent agreement with the theoretical predictions.

All these predictions were obtained by resumming the perturbation series. The natural next step is to look for important physical effects that cannot be seen by any method of resumming the perturbation series. At present, two approaches are being pursued in the search for such effects. One method is to find nonperturbative effects that are present already on the classical level, and the second method is to construct exactly solvable models of quantum field theory including, in particular, models in both two and higher dimensions.

Related topics of physics which have been investigated include the global formulation of gauge fields, approach to equilibrium, radiative processes in QED and QCD, supersymmetry, and lattice gauge theory.

Goals and/or Major Results to Date

They have developed a comprehensive theory for scattering processes at extremely high energies. A number of predictions of this theory, including the increasing total cross sections, the increasing total elastic cross sections, the moving dip, and the rising plateau, have all been later verified experimentally. More recent theoretical results include the possible occurrence of indeterminate-mass particles, dynamic generation of mass, dynamic determination of coupling constants, closed partial differential and difference equation for the Green's functions, a solvable Z_2 lattice gauge theory, classical models of confinement, and a monopole as a short-distance probe.

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1004

HARVARD UNIVERSITY
Cambridge, Massachusetts

Award No.: DE-AC02-76ER03064

Title of Project: Pipkin Group

Person in Charge: F. M. Pipkin

Scientific and Professional Staff: Pipkin, Giles, Hassard, Nickerson, Michael, and Wolinski

Scope of Work

This group was formed at the time the Cambridge Electron Accelerator was being completed. Its first objective was the measurement of wide angle electron-positron pair production using a two arm spectrometer system. The apparatus was subsequently used to study rho, pion, and kaon photoproduction and to measure inelastic electron scattering from carbon. This program was later transferred to Cornell where three different dual spectrometer systems were used to study electroproduction of hadrons. In particular, the pion form factor and inclusive hadron production were measured over a wide kinematic range. This group then collaborated on a FNAL experiment using muons and the CCM spectrometer to study form factors and leptoproduction of hadrons at much higher energies. The group also collaborated on a FNAL experiment studying the scattering of high energy pions and protons from polarized protons.

More recently this group has been an active member of the CLEO collaboration at Cornell and helped to construct the large magnetic detector. This experiment has studied the Upsilon resonances; in particular, they detected bare bottom and analyzed the weak decays of the b quark. Currently the group is participating in the reconstruction of the CCM spectrometer for the investigation of leptoproduction of hadrons in the new Tevatron Muon Beam (Experiment E665). The forward shower counter for the CCM spectrometer is being constructed at Harvard.

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Title of Project: Wilson Group

Person in Charge: R. Wilson

Scientific and Professional Staff: Wilson, Goodman, Kinoshita, MacKay, Hempstead, Kroll, and Schwartz

Scope of Work

The initial work of this group was on electron scattering by protons and deuterons at the CEA. This experiment showed that the electric and magnetic form factors were proportional to each other and that they have a dipole form. In experiments at BNL, the group studied leptonic decays of vector mesons and muon tridents. When the CEA was converted to a colliding beam machine, this group participated in the BOLD experiment. The cross section for the production of hadrons was found to be larger than expected, which was the first evidence for new quarks. After the closing of the CEA, the group turned to the muon scattering program at FNAL with the CCM spectrometer. This program confirmed the breakdown of Bjorken scaling of the nucleon inelastic structure functions. Hadron production by muons was also extensively studied and was found to agree with Feynman scaling as modified by QCD. The final run of this experimental series used nuclear targets and observed nuclear shadowing for $Q^2 < 1$ GeV^2. In a later experiment with this apparatus, the production of charmed mesons by hadrons was studied.

More recently this group has explored the feasibility of neutron antineutron mixing studies at a nuclear reactor. A detailed proposal was submitted for such an experiment at ORNL using a 20 m magnetically shielded flight path and a thin target for observing annihilations.

The group is currently a member of the CLEO collaboration at Cornell, which has studied the Upsilon resonances and detected the existence of bare bottom. They are also participating in FNAL E665, which will study the production of hadrons by muons at Tevatron energies using a rebuilt CCM spectrometer. Finally, the group is helping with the upgrade of the CERN UA1 experiment and, in particular, with the design of a central calorimeter using uranium plates.

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Title of Project: Strauch Group

Person in Charge: K. Strauch

Scientific and Professional Staff: Strauch, Antreasyan, Irion, McBride, and Willians

Scope of Work

This group had its origin in the CEA BYPASS project, where the CEA staff developed an e^+e^- colliding beam facility. They collaborated on the building and running of the BOLD experiment, which made the initial discovery of the large hadron production cross section which was later verified at SPEAR. The group then participated in a CERN ISR experiment which measured dimuon production. Scaling was observed as a function of the variable $m_{\mu\mu}/\sqrt{s}$ and the data were found to be in agreement with the Drell-Yan mechanism.

More recently this group participated in the Crystal Ball experiment at SPEAR studying the production of neutral particles decaying into photons. This experiment has made extensive contributions to charmonium spectroscopy, in particular, establishing the charmed eta state at 2.98

GeV and the observation of various chi states. The Crystal Ball has now been moved to DORIS II where it is being used to study single photon transitions of Upsilon states and two-photon physics. The Harvard group built new luminosity monitors for the relocated experiment.

The group has joined with others in the planning and building of the LEP-3 Experiment for LEP. A full-scale octant of the detector has been set up on the floor of the High Energy Physics Laboratory at Harvard where the muon chambers will be tested.

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Title of Project: Rubbia Group

Person in Charge: C. Rubbia

Scientific and Professional Staff: Rubbia, Rohlf, Winn, Aprile, Geer, Giboni, Phillips, and Worstell

Scope of Work

This group was initially involved in neutrino scattering experiments at Fermilab and Brookhaven. The Harvard-Pennsylvania-Wisconsin experiment at FNAL studied charged current structure functions, confirmed the existence of neutral currents, and observed anomalous dimuon events. At BNL neutral current scattering was further studied and neutrino oscillations were sought. Major parts of both detectors were built by the Harvard group. The group also participated in an ISR experiment studying new particle production and diffractive phenomena and in an internal target experiment at FNAL studying high P_t photons in pp collisions.

Recently this group planned and built a large Cerenkov detector consisting of 800 tons of water 1800' below ground in collaboration with two other institutions. This detector is being used to search for the decay of the proton, in particular those decay modes which include a muon. The subsequent decay of the muon flags such events. Several possible candidates have been observed.

Finally, the group leader has been largely responsible for the proton-antiproton program using the CERN SPS as a colliding beam facility. The Harvard group has now joined the UA1 experiment, participating in the discovery and analysis of the W and Z^0 particles. They will share the responsibility for the upgrading of the central calorimeter using uranium plates.

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HARVARD UNIVERSITY
Cambridge, Massachusetts

Title of Project: Schwitters Group

Person in Charge: R. F. Schwitters

Scientific and Professional Staff: Schwitters, Blocker, Brandenburg, Eaton, Carey, Kearns, St.Denis, and Schaad

Scope of Work

This task began in summer 1979 when Roy Schwitters joined Harvard coming from SLAC. Its initial activity was participation in the continuing Mark II program at PEP. They had primary responsibility for the drift chambers, and in the data analysis they concentrated on the areas of tau physics, algorithms for jet finding, and weak-EM interference effects. A detector for the PEP polarimeter was also designed and built.

The group joined the CDF collaboration at Fermilab where Roy Schwitters is now the overall project manager. The Harvard group has taken on the responsibility together with Brandeis for the design and construction of the Forward/Backward Shower Counters for the detector. They are also actively involved in the development of analysis software for the project and expect to play a major role in the physics analysis when proton antiproton collisions at 2 TeV begin in 1986.

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Title of Project: Theory Group

Person in Charge: R. J. Glauber

Scientific and Professional Staff: Glauber and others

Scope of Work

The principal investigator of this task developed the quantum theory of optical coherence and the theory of the photon statistical properties of laser fields as applications of quantum electrodynamics. He also developed the theory of coherent and incoherent multiple diffraction phenomena for high energy hadron-nucleus collisions. More recently the group has devoted attention to various radiation processes fundamental to the new field of quantum optics and to the properties of devices such as quantum mechanical amplifiers fundamental to quantum electronics. Extensive studies have also been made of new approaches to hadronic diffraction phenomena. In particular, a program of phenomenological analysis of high energy proton-proton and proton-antiproton cross sections has been begun. Work also continues on the application of the new asymptotic diffraction theory to proton-nucleus collisions at intermediate energies.

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HARVARD UNIVERSITY
Cambridge, Massachusetts

Award No.: DE-FG02-84ER40171

Title of Project: Analysis of UA1 Data at Harvard

Person in Charge: J. W. Rohlf

Scientific and Professional Staff: J. W. Rohlf

Scope of Work

Data from experiment UA1 (Aachen, Annecy, Birmingham, CERN, Harvard, Helsinki, Kiel, Queen Mary College, London, NIKEF, Paris, Riverside, Rome, Rutherford, Saclay, Vienna, Wisconsin Collaboration) on proton-antiproton collisions at a center-of-mass energy of 540 GeV will be analyzed at Harvard University. This will give insight on the basic structure of matter and subatomic forces.

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UNIVERSITY OF HAWAII
Honolulu, Hawaii

Award No.: DE-AT03-83ER40103

Title of Project: Neutrino Physics at Fermilab (E632)

Persons in Charge: V. Z. Peterson and F. A. Harris

Scientific and Professional Staff: R. J. Cence, F. A. Harris, M. D. Jones, V. Jain, M. W. Peters, V. Z. Peterson, and A. Koide

Scope of Work

E632 is the first 15-foot bubble-chamber experiment scheduled (late 1984) for the Fermilab wide-band neutrino beam. It is a European-U.S. collaboration involving 12 institutions, and the new equipment required to upgrade the hybrid bubble chamber represents contributions from Europe as well as the U.S. Holographic photography, involving a multi-joule pulsed ruby laser of microsecond pulse length, is a feature of the new equipment. Major improvements in the neutrino beamline are required for this and other experiments. New electronic detectors for muon identification and bubble-chamber event prong tagging have been constructed at CERN and at Fermilab and are being installed. This experiment is a survey of interactions produced by the higher energy neutrinos produced by the 800-1000 GeV protons from the Tevatron. The visual method provides the opportunity to study neutrino interactions in detail, to detect visible charm and beauty decays as well as strange particle decays, and to correlate phenomena involving leptons and hadrons in a single event.

Goals and/or Major Results to Date

A primary goal is to detect the decay of short-lived particles, using holography with resolution 100 microns or better. At Hawaii a holographic measuring machine capable of 20 micron accuracy is being built. Using the External Muon Identifier (EMI) and Internal Picket Fence, in conjunction with the neon-hydrogen bubble chamber, they expect to establish the principal characteristics of high-energy neutrino events. Hawaii personnel have played key roles in the design of the EMI, and the on-line and off-line software development for E632.

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Title of Project: e^+e^- Collisions at the SLAC Linear Collider

Persons in Charge: R. J. Cence and V. Z. Peterson

Scientific and Professional Staff: R. Cence, F. Harris, S. Parker, V. Peterson, and D. Yount

UNIVERSITY OF HAWAII
Honolulu, Hawaii

Scope of Work

The Mark II detector will be the first detector to be run in the only interaction region of the Stanford Linear Collider (SLC). e^+e^- collisions of 50 + 50 GeV are expected in late 1986. The Hawaii group is one of about six groups in the Mark II collaboration and is currently helping to upgrade the Mark II detector for SLC experiments. A special project of the Hawaii group is the development of a secondary vertex detector using silicon microstrip elements, plus VLSI microchip readout electronics. This will make it feasible to utilize one of the major advantages of the SLC: finely focussed beams interacting within a cross section only a few microns in diameter. The positioning of several layers of high-resolution detector close to the SLC interaction point, together with outer layers of drift chambers, promises to make the Mark II detector an even better device for measuring the decay distances of short-lived particles.

Goals and/or Major Results to Date

The primary goal of the SLC is to produce Z^0 particles: the expected yield is over 10^6 Z^0 events annually. Decays of the Z^0 are of great interest, and the Mark II's ability to track the decay products (including very short-lived secondary decays) will be important. Measuring the width of the Z^0 is one way to determine the number of neutrino types. Detection of the Higgs particle is another goal.

Progress in development of silicon microstrip detectors is very encouraging. Cooperating with CERN experts, Hawaii now has the first batch of silicon strips for radiation tests. A successful design of the VLSI microstrip has been completed at the Stanford Integrated Circuit Laboratory, with major participation from Hawaii and CERN personnel. It appears that the chip design has wide applications in particle physics.

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Title of Project: Deep Underwater Muon and Neutrino Detection (DUMAND)

Persons in Charge: V.Z. Peterson, J.G. Learned, and V.J. Stenger

Scientific and Professional Staff: J. Babson, R. Cady, S. Dye, and J. Learned, D. O'Connor, V. Peterson, and V. Stenger

Scope of Work:

DUMAND (Deep Underwater Muon and Neutrino Detection) is an international collaboration in nonaccelerator physics: neutrinos and muons from cosmic rays and astrophysical sources are the particles to be detected by a giant underwater array of optical (and acoustic) detectors. Observations of neutrinos from astrophysical point sources is a primary goal. DUMAND is a logical extension of the deep mine detectors which have searched for "cosmic" neutrino interactions for many decades. DUMAND is related in technique to the water-Cerenkov detector experiments on proton decay now running in the U.S. and Japan. In the U.S., the five groups supported by DOE (Hawaii, Purdue, Wisconsin, CalTech, and UC-Irvine) are joined by Vanderbilt (NSF) and Scripps (ONR) in pursuing various tasks related to the 756-module detector, the data and power link to shore, and the analysis of the events. Cosmic ray groups from Bern, Kiel, and Tokyo round out the collaboration. Hawaii is the center of activity due to its natural advantages of deep, clear water close to land and the active support of the University of Hawaii.

Goals and/or Major Results to Date

After a three-year feasibility study and a successful proposal for funding of Stage I (a Short Prototype String of 8 modules), the group is now completing electronic design and assembling the prototype modules of large phototubes encased in glass pressure-spheres. A test tank provides facilities for calibration of the (16" diameter) photon detectors. Ocean deployment of test modules has provided realistic measures of the optical background, and Monte Carlo simulations predict the expected results of late 1984 ocean tests. Funding is being sought for the long (40 km.) electro-optic cable to shore required to bring 1 GHz of data from the full array back to shore.

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Title of Project: Theoretical High Energy Physics

Person in Charge: S. Pakvasa

Scientific and Professional Staff: E. Ma, S. Pakvasa, W.A. Simmons, S. F. Tuan, K. Babu, and X.-Y. He

Scope of Work

Participants in this program pursue basic theoretical physics research in various areas of high energy physics. There is an active visiting and collaborative program with H. Sugawara of KEK, Japan, and with the University of Wisconsin phenomenology group.

The interests and research of the group range from pure theory to phenomenology. There is great interest in interpreting new experimental data as well as building models which make definitive predictions.

UNIVERSITY OF HAWAII
Honolulu, Hawaii

Goals and/or Major Results to Date

During the last year, members of the group produced important results in the following topics: fermion masses and mixings, existence of the Higgs particle, uniqueness of supersymmetry, CP-nonconservation in standard and nonstandard models, possible existence of glueballs and other exotic states, etc. The possible deviation from the standard model is of special interest as an indicator of future direction for theory and the current data, especially from the $\bar{p}p$ collider, will be watched closely.

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1013

HOUSTON AREA RESEARCH CENTER
The Woodlands, Texas

Award No.: DE-AC02-84ER40155

Title of Project: Design and Modeling of Warm/Cold Iron Accelerator-Quality Superferric Magnets

Persons in Charge: F. R. Huson and P. M. McIntyre

Scientific and Professional Staff: H. Bingham, J. Colvin, M. Davidson, A. Dragt, J. Greenough, L. Healy, S. Heifets, H. Hinterberger, B. Huguelet, M. Kobayashi, G. Lopez, W. MacKay, D. Neuffer, S. Pissanetzky, R. Rocha, R. Ryne, W. Schmidt, R. Stegman, T. Tominaka, R. Wolgast, J. Zeigler

Scope of Work

The design and modeling of warm iron (2.3 Tesla) and cold iron (3.0 Tesla) accelerator quality magnets for potential use in the proposed Superconducting Super Collider (SSC). These R&D activities include: (1) complex accelerator design calculations to ensure that these magnets are optimized for a 20 TeV proton-proton collider; (2) stress analyses and other appropriate engineering computations for components of the magnets; (3) cryogenic calculations to study special refrigeration schemes for magnet systems based on these designs and the power required for refrigeration; and (4) electrical studies of the associated magnet power supply and quench protection systems. The effort also includes fabrication of small models of each type of magnet to adequately test design features, tolerances, quench limits, and improved methods of fabrication and assembly. Detailed performance tests include: (1) measurement of the multipole components of the magnetic field and comparison with predictions based on extensive computer simulations; (2) measurement of the effects of persistent currents; and (3) heat leak measurements. In addition, those activities will be carried out as are required to interface with and support R&D on the SSC being carried out elsewhere, including providing cost analyses and estimates for the use of superferric magnets in the SSC, accelerator physics affecting the use of superferric magnets, and providing expertise on superferric magnet technology to other R&D groups studying the SSC.

Goals and/or Major Results to Date

Working space has been obtained and a staff of scientific, professional, technical, and administrative personnel has been assembled. Shop facilities have been put in place. Cryogenic test facilities for both 1 meter cold iron and 3 meter sections of warm iron magnets (for thermal properties only) are under construction.

Two 1 meter cold iron magnets have been designed and fabricated and are undergoing test. The preliminary results are better than expected; both achieved the full field of 3.0 Tesla and required raising the He bath temperature to force a quench of 10 kiloamps.

Construction has been started on 8 meter cold iron magnets. Industry is being involved.

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UNIVERSITY OF ILLINOIS
Chicago, Illinois

Award No.: DE-FG02-84ER40169

Title of Project: Parton Dynamics in Hadronic Precesses

Person in Charge: U. P. Sukhatme

Scientific and Professional Staff: U. P. Sukhatme

Scope of Work

To get a better understanding of the dynamics of quarks and gluons in hadronic interactions by studying multiparticle production in soft hadronic collisions in a dual parton model framework and the fragmentation of composite, spatially extended colored systems.

Continuation of an ongoing program of development and applications of shifted large N expansions in quantum mechanics and quantum field theory.

Goals and/or Major Results to Date

Several aspects of the dual parton fragmentation model for low transverse momentum multiparticle production in hadronic collisions have been elucidated. In particular, it has been verified that the dual parton model correctly reproduces recently obtained two particle inclusive distributions and particle ratios in the central region of pp and $p\bar{p}$ collisions. This work sheds light on the dynamics of partons in a hadronic collision since it strongly indicates that a valence quark from each initial hadron is "held back" with a small momentum fraction. Also, the dual parton approach has been extended to include diffraction dissociation and the consequences on inclusive pion production in pp interactions have been studied. He has investigated the virtues and limitations of logarithmic perturbation theory, which is often a much simpler alternative to standard Rayleigh-Schrodinger perturbation theory. Finally, he has developed and studied the shifted 1/N expansion for the energy eigenstates in nonrelativistic quantum mechanics. The results provide an accurate, rapidly convergent, powerful new way of handling any spherically symmetric potential.

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1015

UNIVERSITY OF ILLINOIS
Chicago, Illinois

Award No.: DE-FG02-84ER40173

Title of Project: Gauge Theories and Their Consequences

Person in Charge: W.-Y. Keung

Scientific and Professional Staff: W.-Y. Keung

Scope of Work

Selective topics will be pursued to further the theoretical understanding of particle interactions. Specific topics will include such studies as the production of heavy unstable neutrinos from weak boson decays; amplitudes for Majorana Fermions; the enhancement of Higgs production in SUSY; signatures for heavy quark productions; testing of the standard model in high precision; rare decays of the B-mesons; direct photon spectrum from the upsilon decays; W Boson decays into the Psi/J-like particles; and, fermion-monopole systems.

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UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN
Urbana, Illinois

Award No.: DE-AC02-76ER01195

Title of Project: Neutrino Oscillation

Person in Charge: T. O'Halloran

Scientific and Professional Staff: E. O'Brien, K. Reardon, and S. Salman

Scope of Work

The goal of this experiment is to search for neutrino oscillations. The initial phase of the experiment will be to search for the $\nu_\mu \rightarrow \nu_e$ transitions. This phase of the experiment will be sensitive to Δm^2 of 0.03 eV^2 and $\sin^2 2\alpha$ of order 10^{-3}. This will represent an order of magnitude improvement over current limits (March 1984). The idea that neutrinos could oscillate between states of different flavor was suggested several years ago by Pontecorvo. If this phenomenon were found to occur, it would have profound implications in areas of physics ranging from particle physics to cosmology. It would demonstrate that neutrinos have non-zero mass and are, therefore, not pure helicity states. It would also show that lepton numbers for the different flavors are not independently conserved. These facts would impact upon the form of current theories, as well as upon the question as to whether the universe is open or closed.

Goals and/or Major Results to Date

At the present time they are installing the detector at Brookhaven National Laboratory, and they are scheduled to receive beam in November, 1984. They see no reason why the experiment will not be ready to receive beam. The primary goal, therefore, is to extend the limits on $\nu_\mu \rightarrow \nu_e$ transitions to $\Delta m^2 \sim .03$ and $\sin^2 2\alpha \sim 10^{-3}$ during the scheduled running periods in 1984-1985.

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Title of Project: Neutral Beam Experiments at Fermilab

Persons in Charge: J. Wiss and G. Gladding

Scientific and Professional Staff: J. Busenitz, M. Diesburg, J. Filaseta, L. Koester, T. Kroc, C. Olszewski, C. Shipbaugh, and B. Tripsas

Scope of Work

This group performs neutral beam experiments at Fermilab using a multiparticle spectrometer with substantial particle identification capabilities. They have studied the interactions of high energy neutrons and high energy photons. Their neutron production experiment is concentrating on the production dynamics of charm particle hadron production. Their photoproduction experiments have studied the production of the ρ, ω, ϕ, ψ, ψ' vector mesons at high energies and they have studied the production of charmed mesons and baryons. Their future photoproduction experiment will extend these measurements to still higher energies and will study the production of the γ and beautiful baryons and mesons.

Goals and/or Major Results to Date

They have observed and studied the photoproduction of the D^{*+} and Λ^+_c at an average photon energy of 120 GeV. They have observed the photoproduction of the $\rho' \rightarrow \pi^+\pi^-$ for the first time. They have measured the energy dependence of the ρ, ϕ, ω, ψ, ψ' cross section from 70 to 200 GeV from H_2 and D_2 targets and have studied the fraction of vector meson events which are produced elastically off of protons using a recoil detector.

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Title of Project: e^+e^- annihilations at SLAC

Person in Charge: R. Eisenstein

Scientific and Professional Staff: G. Gladding, J. Thaler, A. Wattenberg, R. Dobinson, R. Downing, W. Wisniewski, J. Becker, G. Blaylock, S. Plaetzer, C. Simopoulos, A. Spadafora, and B. Tripsas

Scope of Work

This group pursues two areas of research. One area consists of the study of the physics of gluons, charmed quarks, and heavy leptons; all are accessible to the Mark III experiment at SPEAR. The other area consists of the study of the Z^0 boson, testing Weinberg-Salam in its weak decays and also investigating the properties of the particle into which it decays, including searching for the top quark, new kinds of neutrinos, and evidence for supersymmetry. They are preparing to help build a detector, the SLD, to run at SLC for this purpose.

Goals and/or Major Results to Date

The Mark III group has presented results on the radiative decays of the ψ meson. These include the measurement of the spin and parity of the η_c meson, the study of the ι and θ glueball candidates, and the discovery of a new, narrow resonance at 2.2 GeV. They are also now achieving their first results on charmed meson decays, verifying that the Cabibbo-suppressed decays $D^0 \rightarrow K^+K^-$ and $D^0 \rightarrow \pi^+\pi^-$ do not have equal rates. They plan to set stringent upper limits on D^0-D^0 mixing and CP violation.

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN
Urbana, Illinois

The SLD project is just beginning. They plan to build the trigger electronics and various diagnostic packages for the detector.

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Title of Project: FASTBUS Hardware Studies

Person in Charge: R. Downing

Scientific and Professional Staff: R. Downing

Scope of Work

They are involved in the application of new technologies for use in FASTBUS systems.

Gate arrays have been studied and general purpose FASTBUS slave interfaces have been proposed. These designs have been thoroughly examined by Illinois and other laboratories. Production is dependent upon lab or large experiment use of these parts.

Methods of cooling high powered systems have been investigated using air, water, and air/water designs. A significant reduction in fan noise has been accomplished by proper choice of components and sound absorbent material.

Serial communication systems have been prototyped using Ethernet and fiber optics. Results of these tests may lead to the implementation of serial standards in the FASTBUS specification. Such serial standards are alluded to in the current document but left undefined.

Goals and/or Major Results to Date

Alternates to gate arrays will be developed using hybrids and/or PAL's. They will work with a group at CERN to develop some "standard" interfaces. These will ease the design problems of potential FASTBUS users.

They are still investigating cooling of very high powered IC's. They feel some simple solutions are possible which will allow users to design electronics similar to conventional air-cooled systems.

Of particular importance has been the development of general purpose FASTBUS equipment and techniques as a service to the entire FASTBUS user group. They have provided easy methods to interface to FASTBUS. Some developments from this group include the Segment Interconnect, cable segment hybrids, gate array interfaces, PAL interfaces, hybrid interfaces, Ethernet and fiber optic FASTBUS links, and cooling of high powered FASTBUS cards.

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UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN
Urbana, Illinois

Title of Project: Charged Particle Beam Experiments and the Collider Detector at Fermilab

Person in Charge: L. Holloway

Scientific and Professional Staff: G. Ascoli, S. Cihangir, I. Karliner, L. Koester, U. Kruse, R. Sard, J. Simaitis, D. Smith J. Bellinger, T. Graff, W. Li, P. Lukens, and T. Westhusing

Scope of Work

This task covers experiments using the Chicago Cyclotron facility at Fermilab for the production by pions and protons of charmonium states and experiments planned for the Collider Detector at Fermilab (CDF).

The object of Fermilab Experiments E-610 and E-673 was to study the hadronic production of charm-anticharm states, in particular the χ, and to observe particles produced in association with ψ/J. The study of these processes enables us to learn something about the quark and gluon content of hadrons and to assess the relative importance of different charmonium production mechanisms, e.g., quark-antiquark fusion or gluon-gluon fusion.

The Illinois group has primary responsibility for the CDF central muon detection system. The purposes of this detection system are to provide precise position measurements of muons which penetrate the central electromagnetic and hadron shower calorimeters and to provide a signal suitable for triggering on potentially interesting events containing muons.

Goals and/or Major Results to Date

Analysis of the data obtained in E-610 is complete and that for E-673 is nearing completion. The main interesting physics result is that the relative amounts of various χ states seem to differ depending on whether the incident beam particle is a pion or a proton, thus indicating more than one production mechanism. Furthermore, an analysis of the average charge of the hadrons associated with J/ψ final states does not agree with naive production models, indicating a more complex dynamic mechanism.

The assembly line for the fabrication of drift chambers for the CDF central muon detector is now in full production. The goal is to be finished in time for the May 1985 $p\bar{p}$ test run. The design and testing of various associated electronics is proceeding satisfactorily.

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UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN
Urbana, Illinois

Title of Project: Brown Group

Person in Charge: R. M. Brown

Scientific and Professional Staff: S. Coffman, R. Downing, J. Kohlmeier, D. Lesny, M. Long, V. Simaitis, and J. Wray

Scope of Work

This task covers digital systems research and design plus computer and other services in support of current and future high energy experimental requirements. The group operates a DEC 10 and VAX-11/780 facility (currently being upgraded to a VAX-11/780 and /785 facility) with time-sharing provided to labs and offices in Urbana. It also has developed multiplexed links to the computing facilities at Fermilab and SLAC.

Aside from providing design support to on-going experiments, the group has been intensively involved in developing basic software and hardware standards and elements for FASTBUS data acquisition and control systems.

Goals and/or Major Results to Date

The group has been a contributor of major equipments to the experimental task groups at Illinois. Notable examples in recent years include the Mark III trigger at SLAC and the 8 MB data buffer system on Experiment 400 at FNAL. Future work will involve the muon detector and other systems for CDF and the trigger for the proposed SLD at SLAC.

In addition, the group has made extensive contributions in developing software and hardware elements and standards for FASTBUS data network systems. Hardware developments are covered in a separate FASTBUS hardware task summary. The FDL diagnostic language designed by this group has been implemented on several DEC computers and is used to create diagnostic and engineering test programs. A Software Resource Guide has been developed and distributed extensively.

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Title of Project: Theoretical and Phenomenological Studies in Elementary Particle Physics

Person in Charge: L. M. Jones

Scientific and Professional Staff: C.-K. Ng

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN
Urbana, Illinois

Scope of Work

This task covers theoretical and phenomenological computations in elementary particle physics. The long range goal is to achieve a quantitative understanding of high energy reactions. At present, emphasis is being placed on applications of QCD and properties of quark and gluon jets. Other calculations for strong and electromagnetic processes may be undertaken.

Almost all the actual advances made during this year concern calculations of jet quantities. The collaboration involved here includes graduate student C.-K. Ng at Urbana, Professor Roger Migneron of the University of Western Ontario, his graduate student at Western, Sowmya Naranayan, and Bruno Crespi of the University of Trento in Italy.

Other phenomenological calculations will be pursued as more students join the group. The number of possible topics here is very large, including (but not limited to): a) charm production in the forward direction of hadronic interactions; b) coupling of glue states to quarkonia; c) Skyrmion model of the proton; and d) predictions about interesting properties of the bulk of collider data--the forward "spectator jet."

Goals and/or Major Results to Date

They have found new "backward-moving" Altarelli-Parisi equations in which the mass of the parton under observation evolves down. These equations express analytically the same process as occurs in Monte Carlo evolution programs for jets. Longitudinal and transverse degrees of freedom can be separated; this makes computations of transverse momentum properties much simpler.

Cho-Kuen Ng has been studying various features of Monte Carlo programs for jet evolution in the light of analytic calculations. They believe they understand the reasons for differences (in colorless cluster average masses) between previously published analytic and Monte Carlo calculations. Naranayan has derived new equations for the behavior of the various semi-inclusive jet propagators at small x.

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ILLINOIS INSTITUTE OF TECHNOLOGY
Chicago, Illinois

Award No.: DE-AC02-80ER10712

Title of Project: Theoretical Studies in Elementary Particle Physics

Person in Charge: J. C. Collins

Scientific and Professional Staff: J. C. Collins, P. W. Johnson, and W.-K. Tung

Scope of Work

Currently the work is aimed at a better understanding of QCD (Quantum Chromodynamics), which is the theory of strong interactions. They have discovered and continue to develop methods to extend greatly the range of processes to which perturbative (weak-coupling) methods can be reliably applied. They are also working on numerical calculations of cross sections using these methods. Another project concerns the numerical solution of the Dyson-Schwinger equations for QCD.

Goals and/or Major Results to Date

Over the past few years a collaboration of Collins with D. Soper (University of Oregon) and G. Sterman (SUNY, Stony Brook) has produced expansions for processes such as the transverse momentum distribution for dimuon production in hadron collisions. The ultimate aim is to understand the relation to the non-perturbative regime.

They also aim at reliable numerical predictions testing the validity of QCD.

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INDIANA UNIVERSITY
Bloomington, Indiana

Award No.: DE-AC02-84ER40125

Title of Project: Elementary Particle Physics

Person in Charge: R. M. Heinz

Scientific and Professional Staff: S. Ahlen, D. Blockus, B. Brabson, R. Crittenden, A. Dzierba, S. Gray, R. Heinz, T. Marshall, H. J. Martin, H. Ogren, D. Rust, A. Snyder, D. Zieminska, and A. Zieminski

Scope of Work

The Indiana University high energy physics group is performing experiments at Fermilab, SLAC, and Brookhaven. The Fermilab program is based on Experiments E-557 and E-672, which are designed to study jet and dimuon production utilizing the Multiparticle Spectrometer. The High Resolution Spectrometer (HRS) was built at SLAC's PEP accelerator for use in a major study of electron-positron collisions. The HRS detector, having the highest resolution of any such detector at a high energy e^+e^- storage ring, is being used to explore jets, to study production of strange and charmed mesons, and to measure direct photon production. At Brookhaven the group is studying characteristics of the E meson in Experiment E-771. This experiment will permit a high statistics analysis to be made to determine if the E meson is indeed a glueball state. Finally, they may search for magnetic monopoles under the Gran Sasso Mountain in Italy.

Goals and/or Major Results to Date

The group has studied D and D^* production using the HRS at SLAC's PEP accelerator. At Fermilab jet-like structure was observed in high transverse energy events in 400 GeV/c proton-proton collisions. Also at Fermilab, K^* production was measured using 50, 100, and 175 GeV/c π^- and K^- beams interacting with hydrogen; A_2 production was also observed in this Fermilab experiment. The gluon structure function of the pion was measured in an experiment at CERN.

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Title of Project: Theoretical Particle Physics

Persons in Charge: A. W. Hendry, D. B. Lichtenberg, and D. H. Weingarten

Scientific and Professional Staff: M. Anselmino, L. Clavelli, A. W. Hendry, D. B. Lichtenberg, W. Namgung, and D. H. Weingarten

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INDIANA UNIVERSITY
Bloomington, Indiana

Scope of Work

The members of the group are principally studying the properties and interactions of mesons and baryons using the theory of quantum chromodynamics (QCD) and approximations to this theory. The principal technique used at high energy is perturbation theory, but at low energy potential models motivated by QCD and lattice versions of QCD are also used. The group also does research on generalizations of the standard model of elementary particles, including investigating grand unified theories, the possibility that quarks are composite particles, and quantum gravity on a lattice.

Goals and/or Major Results to Date

The group has succeeded in calculating masses of mesons and baryons in both potential models and in lattice QCD. The calculated masses are in fairly good agreement with the experimental values. Also, the spin dependence of proton interactions, the properties of hadron jets, heavy quark production cross sections, and the structure functions of nucleons in nuclei have been calculated with rather good success.

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INSTITUTE FOR ADVANCED STUDY
Princeton, New Jersey

Award No.: DE-AC02-76ER02220

Title of Project: Problems in Particle Theory

Persons in Charge: S. L. Adler and R. F. Dashen

Scientific and Professional Staff: G. Bhanot, F. David, S. Gupta, H. Hamber, V. P. Nair, A. Niemi, N. Seiberg, A. Strominger, and J. Breit

Scope of Work

This project supports members of the Institute for Advanced Study working on problems in high energy theory. The specific problems investigated depend on the individuals supported from year to year. Recently, the emphasis has been on model field theories, grand unification phenomenology, supersymmetric grand unification schemes, lattice gauge theories and related numerical methods, perturbative calculations in QCD, and inflationary universe cosmology.

Goals and/or Major Results to Date

Results of research on the above topics are available as Institute for Advanced Study preprints and are published in various scientific journals. Significant advances have been made each year in several of the general areas under study.

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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
Trieste, Italy

Award No.: DE-FG01-82ER40067

Title of Project: Research in High Energy Theoretical Physics

Person in Charge: A. Salam

Scientific & Professional Staff: L. Bertocchi, N. Craigie, G. Furlan, R. Iengo, and J. Strathdee

Scope of Work

The International Centre for Theoretical Physics is an institution belonging to the International Atomic Energy Agency and UNESCO, whose main goal is to foster research in physics in developing countries. In the field of high energy physics, this is done through either long research stages of scientists at the Centre, or through research workshops and topical conferences and meetings. A large number of U.S. scientists participate every year, both in the research workshops and in the topical meetings and conferences.

Goals and/or Major Results to Date

In the last years, the following activities have been organized:

1979	Second Marcel Grossmann Meeting on the Recent Developments of General Relativity (5-11 July)	370 participants
	Summer Workshop on Theoretical Physics (12 July - 3 August)	136 participants
	Topical Meeting on Confinement and Related Problems (26 - 28 November)	54 participants
	Research in Elementary Particle Theory (throughout the year)	148 participants
1980	Seventh Trieste Conference on Elementary Particle Physics (30 June - 3 July)	153 participants
	Session on Development in Grand Unified Theories (25 -29 August)	69 participants
	Research in Elementary Particle Theory (throughout the year)	180 participants

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
Trieste, Italy

1981	Spring School and Workshop on Supergravity (22 April - 6 May)	133 participants
	Conference on Differential Geometric Methods in Theoretical Physics (30 June - 3 July)	118 participants
	Meeting on Monopoles in Quantum Field Theory (11 - 15 December)	123 participants
	Research in Elementary Particle Theory (throughout the year)	217 participants
1982	Summer Workshop in Particle Physics (21 June - 31 July)	77 participants
	September School and Workshop on Supergravity and Supersymmetry (6 - 18 September)	161 participants
	Workshop on Non-Perturbative Field Theory & QCD (17 - 21 December)	90 participants
	Research in Elementary Particle Theory (throughout the year)	200 participants
1983	Topical Conference on Radiative Corrections in $SU(2)_L \times U(1)$ (6 - 8 June)	26 participants
	Summer Workshop in Particle Physics (20 June - 31 July)	95 participants
	Research in Elementary Particle Theory (throughout the year)	121 participants

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IOWA STATE UNIVERSITY
Ames, Iowa

Award No.: DE-AC02-80ER10774

Title of Project: Very High Energy Gamma Ray Astrophysics

Person in Charge: R. C. Lamb

Scientific and Professional Staff: R. C. Lamb and D. F. Liebing

Scope of Work

The scientific goals of this project are to discover and study by means of gamma ray astronomy those regions of the universe where particles are accelerated to extreme energies ($\gtrsim$ 1 TeV) and to improve the sensitivity of detection equipment in this energy range. Pioneering discoveries in this area have shown that rapidly rotating neutron stars and objects whose fundamental nature is not yet understood are capable of such particle acceleration.

The atmospheric Cerenkov technique provides a unique and potentially sensitive view of the universe in the region 10^{11} to 10^{14} eV. Iowa State University with the Smithsonian; University College, Dublin; University of Hawaii; and Durham University are collaborating on the development of an improved sensitivity Cerenkov "camera" which forms a two-dimensional image of the Cerenkov signal in the focal plane of the Smithsonian's Whipple Observatory 10 m reflector. Iowa State's contributions are principally in four areas: observations, development of an auxiliary 3 m reflector for eventual "steroscopic" imaging, electronics, and data analysis.

Goals and/or Major Results to Date

They have detected photons with energies in excess of 500 GeV from Cygnus X-3, an X-ray binary source. This source, recently observed by air shower groups at 1000 to 10,000 TeV, may be the archetypical source of cosmic rays.

The major goal is to demonstrate the ability of the camera to detect gamma ray sources fainter by a factor of 10 than those presently seen.

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JOHNS HOPKINS UNIVERSITY
Baltimore, Maryland

Award No.: DE-AC02-76ER03285

Title of Project: Research in Theoretical Physics

Person in Charge: G. Domokos

Scientific and Professional Staff: G. Domokos and S. Kovesi-Domokos

Scope of Work

Participants in this program pursue basic theoretical physics research in high energy physics. There is a visiting theorist program: theorists from various institutions in the U.S. and abroad are invited for short terms (typically two to three months) to share their results and participate in the research. The basic problem the group is investigating is a possible structure of matter beyond the presently known constituents, electrons, various kinds of quarks, etc. While the existence of such a substructure has been repeatedly suggested in the past, there is no satisfactory theory yet for its description. The purpose is to search for acceptable models which explain the puzzles left behind by presently popular theories, such as the repetition of "generations" of constituents (e.g. the electron, muon, tau-lepton). In pursuing this work, active contact is being maintained with high energy experimental physicists at this university and elsewhere, in order to search for experiments which could uncover a substructure of matter.

Goals and/or Major Results to Date

Participants in the program were engaged in and produced results in theories which go beyond the generally accepted, "standard model" of elementary particle interactions, such as supersymmetric theories based on the assumption of a space having more than three dimensions (originally proposed by Kaluza and Klein) and in the theory of approximate symmetries (dynamically broken symmetries) of elementary particle interactions. In addition, a phenomenological analysis of present experimental data is being carried out in the search for signatures of a possible substructure of matter.

These research topics are of continuing interest as they involve crucial questions at the forefront of our understanding of the structure of matter.

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UNIVERSITY OF KANSAS
Lawrence, Kansas

Award No.: DE-AC02-76ER10528

Title of Project: Particle Theory

Persons in Charge: D. W. McKay and H. J. Munczek

Scientific and Professional Staff: D. W. McKay and H. J. Munczek

Scope of Work

The research interests are: the study of quark and gluon propagators in QCD and the application to hadron mass spectrum calculations; chiral dynamics and the study of the connection between QCD and low energy effective hadronic Lagrangians; the study of anomalous Ward Takahashi identities in the path integral approach.

Regular discussions on phenomenology are held with experimental colleagues at Kansas, with a weekly joint seminar focusing on topics of mutual interest.

Goals and/or Major Results to Date

Treatment of the relativistic bound state problem has been improved and a good overall description of hadron masses with very few parameters achieved. Scalar fields have been systematically included in non-linear chiral dynamics for the first time, and the SU (3) breaking at vertices successfully parameterized. Questions raised about the calculation of anomalies in the path of integral formalism have stimulated interest in the literature.

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LA JOLLA INSTITUTE
La Jolla, California

Award No.: DE-AC03-84ER40182

Title of Project: Research in Theoretical Physics

Person in Charge: R.H.G. Helleman

Scientific and Professional Staff: J. A. Wright and C. R. Eminhizer

Scope of Work; Goals and/or Major Results to Date

The goal of this work is to obtain a more realistic estimate of the beam-beam limit for $p\bar{p}$ (conservative) and e^-e^+ (dissipative) systems. The long-time-stability of most conservative systems depends on the presence of invariant tori in the phase space of the dynamical system. A method has been developed to determine the critical parameter values for which the invariant tori disappear and thereby provide a new estimate for the beam-beam limit of $p\bar{p}$ systems. To date, some critical parameter values have been obtained for both odd and even forces. The stability of most dissipative systems depends on the size and location of basins of attraction, regions of phase space in which all orbits are attracted to one limit orbit. A method using Normal Forms has been developed to determine the size and location of the basins of attraction of the origin and other major resonances of the e^+e^- system.

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LEHIGH UNIVERSITY
Bethlehem, Pennsylvania

Award No.:	DE-AC02-76ER02894
Title of Project:	High Energy Physics Research
Person in Charge:	A. Kanofsky

Scientific and Professional Staff: N. Ackurin, D. Gockley, A. Kanofsky, J. Shieh, and E. Gretzinger

Scope of Work

Lehigh is involved, in collaboration with other institutions, in high energy experiments to study jets formed by hadronic and gamma interactions with protons and heavier nuclei. These experiments (E395, E609, and E683) are performed at Fermilab in the Meson laboratory and in the Proton East laboratory. They enable the differences in jet production between incoming beam type and nuclear target interactions to be studied. Also, the structure of the photon will be studied in experiment E683 (Photon Produced Jets) to be performed in the Proton East tagged photon beam in 1986. These experiments use calorimeter modules for rapid measurement of high p_T events and drift chambers for track reconstruction.

As well, the Lehigh group is developing new types of particle accelerators and beam handling devices using channeling techniques. They are also performing calculations on channeling with Monte Carlo techniques, etc. This work is a continuation of an earlier experiment (E507) on high energy channeling performed at Fermilab. They are constructing an apparatus to study channeling at high energy accelerators and are performing channeling experiments related to high energy applications on the Lehigh 3 MeV Van de Graaff.

The group is also reconstructing an ANL streamer chamber system used by the group in ZGS experiment E406 to study particle nuclei interactions.

They are also involved in studies for the new Superconducting Super Collider, further developing ideas presented in several SNOWMASS 1984 contributed papers.

Also, they are comparing the various existing standard jet Monte Carlo programs and comparing them to experimental results.

Goals and/or Major Results to Date

The goals are to study the structure of hadrons, photons, and nuclei by means of jets; to develop new experimental techniques for particle detection, beam handling and acceleration; and to assist in the development of new accelerators.

LEHIGH UNIVERSITY
Bethlehem, Pennsylvania

They have studied high energy channeling and determined that the behavior scales as predicted by theory from low energy channeling.

They have studied jet production from pions and protons incident on protons and heavier nuclear targets, and have determined the single jet and double jet cross sections, structure functions, and how the cross sections scale with the nuclear size. They have searched for the Berger-Brodsky effect.

In the streamer chamber experiment, Lehigh has obtained measurements on nuclear fragments produced in conjunction with high energy particles incident on nuclei, and have correlated the distributions of various particle types.

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LOUISIANA STATE UNIVERSITY
Baton Rouge, Louisiana

Award No.: DE-AS05-77ER05490

Title of Project: Theoretical Research in Particle Physics

Persons in Charge: R. W. Haymaker and L. H. Chan

Scientific and Professional Staff: R. W. Haymakeer, L. H. Chan, and T. Matsuki

Scope of Work

The research interests of the members of this group include a variety of areas:

1. Dynamical Symmetry breaking without fundamental scalars, chiral symmetry breaking.
2. SU(3) sigma/quark model for low energy dynamics and its relation to QCD and soliton baryons.
3. Studies of GUT phase transitions in the early universe.
4. Hadron phenomenology in quark models with emphasis on charm and other new heavy quarks.

Goals and/or Major Results to Date

Recent results include:

1. A derivation of effective hadron dynamics from quark loop dominance in the SU(3) sigma quark model.
2. General methods for obtaining the momentum expansion of the effective action.
3. Consistent description of electromagnetic mass differences and the successful prediction of $D^+-D^0 = 4.7$ MeV and $D^{*+}-D^{*0} = 3.3$ MeV and the model independent predictions $B^+-B^0 = 2.3 \pm .3$ MeV and $B^{*+}-B^{*-} = -2.0 \pm .3$ MeV.
4. Closed form expression for a bound state effective potential giving a stability requirement for dynamical symmetry breaking.
5. Method to include spontaneously broken chiral symmetry in bag models.
6. An improved treatment of tunneling in the inflationary universe scenario.

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Title of Project: Task B - Experimental Research in Particle Physics

Persons in Charge: R. Imlay and W. Metcalf

Scientific and Professional Staff: R. Imlay, W. Metcalf, V. Sreedhar, A. Fazely, and K. Han

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LOUISIANA STATE UNIVERSITY
Baton Rouge, Louisiana

Scope of Work

Electron-positron collisions are being studied at the Cornell Electron Storage Ring (CESR) in the energy region of the upsilon particles. The apparatus is particularly suited for the detection of leptons and photons. The major elements of the apparatus are sodium iodide and lead glass counters, strip chambers around the beam pipe, and a muon detector. Emphasis is being given to the study of the b quark spectroscopy. They are also preparing for an approved neutrino oscillation experiment at Los Alamos.

Goals and/or Major Results to Date

Measurements of the four lowest Υ particles have been made at CESR. These particles are bound states of the fifth quark (b) and its antiquark. They have measured the $\pi\pi$ decays of both the Υ' and Υ'' as well as electromagnetic transitions among the $b\bar{b}$ states. Enhanced electron, muon, and kaon yields have been observed at the Υ''' consistent with dominant $B\bar{B}$ decay of this resonance. They have begun to assemble equipment for the ν experiment.

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UNIVERSITY OF MARYLAND
College Park, Maryland

Award No.: DE-AC05-76ER02504

Title of Project: High Energy Accelerator and Colliding Beam User Groups

Person in Charge: G. A. Snow

Scientific and Professional Staff: C. Y. Chang, R. G. Glasser, S. Gupta, R. G. Kellogg, S. Kunori, P. Rapp, B. Sechi-Zorn, J.A.J. Skard, A. Skuja, P. H. Steinberg, R. Talaga, S. Wagner, G. B. Yodh, G. T. Zorn, R. Bard, C. Hagelgans, M. H. Schmitt, and Z. M. Wang

Scope of Work

The University of Maryland high energy physics group has been engaged in a variety of experiments on weak, electromagnetic, and strong interactions. These include: e^+e^- collisions at DESY using first PLUTO and now JADE, muon neutrino interactions on deuterium and electrons at Fermilab, electron neutrino interactions on electrons at Los Alamos, and finally hadron nucleon jet and dimuon production at Fermilab. In the future, they will participate in the deep inelastic muon experiment at Fermilab, in the OPAL experiment at LEP in CERN, and in the DO $\bar{p}p$ collider experiment at Fermilab.

In the past decade they have moved from a predominantly bubble chamber analysis group to a fully integrated counter group with good engineering and shop support to supplement their analysis capabilities. They maintain a strong interest in phenomenological theory.

Goals and/or Major Results to Date

They have made important contributions on the intrinsic properties of strange particles, their masses, spins and relative parities; weak interactions of strange hyperons leading to Cabibbo's theory; resonant states; the Ω^- hyperon; the energy dependence of pN total cross sections; the $\nu_\mu e^-$ interaction; the discovery of gluons; the photon structure function; tests of QCD. Their goal is to find signals that will lead the way to a more unified and comprehensive understanding of the elementary particles and their interactions.

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UNIVERSITY OF MARYLAND
College Park, Maryland

Award No.: DE-AS05-78ER05940

Title of Project: Accelerator Research Studies

Person in Charge: M. Reiser

Scientific and Professional Staff: W. W. Destler, W. Namkung, M. Reiser, M. J. Rhee, and C. D. Striffler

Scope of Work

This task is concerned with a study of the effects that are responsible for emittance growth and brightness limitations in the transport and initial acceleration of intense particle beams. An electron beam transport channel consisting of 36 short solenoid lenses is being constructed to study beam behavior and compare experimental data with theoretical predictions.

This task is also concerned with exploration of new acceleration schemes that could have an impact on the design of future particle accelerators. Two intense relativistic electron beam generators (2 MV, 30 kA, 30 ns and 0.8 MV, 100 kA, 100 ns) are being used to study collective ion acceleration by an intense relativistic electron beam. In addition, a compact pulsed power plasma focus device has been developed for the generation and study of very short, low-emittance electron and ion beams. Theoretical studies in support of the experiments in both tasks are being pursued in house and in collaboration with outside groups.

Goals and/or Major Results to Date

The first stage (12 lenses) of the electron beam transport channel has been completed. 100 percent transport efficiency with very little emittance growth has been achieved over a wide range of solenoid focusing strength in the 12 periods. Studies of the effects of lens aberrations and space-charge (nonlinearities, instabilities) are in progress.

Many ion species from H to Xe have been accelerated by collective effects to energies as high as 5 MeV/nucleon. Ongoing efforts are aimed at obtaining an understanding of the underlying physics and the development of a slow-wave structure to control and enhance the energy gain. In the plasma focus device, charge and energy distribution of ion species are being measured and compared with theoretical models.

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UNIVERSITY OF MARYLAND
College Park, Maryland

Title of Project: Study of Microwave Sources and Parameter Scaling for High-Frequency Linacs

Persons in Charge: V. L. Granatstein and M. P. Reiser

Scientific and Professional Staff: C. Striffler, J. McAdoo, D. Welsh, A. Drobot, A. Mondelli, D. Chernin, and P. Vitello

Scope of Work

Work in this task is motivated by the fact that the size and cost of high-frequency linacs should be reduced significantly by operating at a shorter wavelength, λ, than in present designs. The present program entails study of the feasibility of a high peak power gyrotron as an rf source for a high-frequency linac in the range 5-15 GHz. Also included is a study of the scaling of beam physics and system parameter with frequency.

The first stage involves a one-year study of both possible microwave sources (phase-locked gyrotron oscillator or gyroklystron amplifier) and beam physics issues to determine an optimum frequency for a 1 TeV accelerator driven by gyrotrons with individual peak power rating of 300 MW. Specific design of an intermediate power gyrotron (10-35 MW) at the optimum frequency will also be carried out, and experiments on an existing lower power gyrotron oscillator will test the efficiency of phase locking.

The second stage is a two-year effort involving construction and testing of a 10-35 MW phase-coherent, efficient source at the chosen frequency. Stage three involves the development of a 300 MW linac prototype gyrotron and would be carried out primarily by a major microwave tube company and/or SLAC with the University of Maryland participating as consultant.

Goals and/or Major Results to Date

A numerical study of a two-cavity 9 GHz, 300 MW gyroklystron amplifier has been initiated and preliminary results show an efficiency of 37 percent and a gain of 25 dB. Possibilities of improving this design by utilizing more than two cavities and making other changes will be investigated. Design of the input coupler and phase diagnostics for a phase locking study on an available 100 GHz, 5KW gyrotron is also in progress.

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UNIVERSITY OF MARYLAND
College Park, Maryland

Award No.: DE-AS05-80ER10666

Title of Project: Charged Particle Beam Transport

Person in Charge: A. Dragt

Scientific and Professional Staff: A. Dragt, R. Gluckstern, F. Neri, E. Forest, L. Healy, E. Opp, and R. Ryne

Scope of Work

A new method has been developed for the description and computation of charged particle beam transport. This method exploits the Hamiltonian nature of the equations of motion with the aid of Lie algebraic tools. These tools, in addition to providing a concise and powerful theoretical procedure for describing and evaluating nonlinear effects, are computationally fast and require relatively little storage. This method is also expected to provide a new theory of nonlinear structure resonances in periodic machines and of the effect of the beam-beam interaction in colliding beam machines. Finally, the method is also applicable to problems such as the design of electron microscopes, microprobes, and low energy wide acceptance spectrometers.

Goals and/or Major Results to Date

On the basis of this new method, a numerical charged particle beam transport program, MARYLIE, has been produced. Initial studies show that MARYLIE gives results comparable in accuracy to those obtained by careful numerical integration, and at speeds comparable to or better than those achieved by present less accurate codes such as TRANSPORT and PATRICIA. For example, in a large machine such as the proposed Superconducting Super Collider (SSC), it appears to be possible to compute with MARYLIE the effect of all lattice elements between successive interaction points using a single map. Thus, MARYLIE is an ideal tool for the calculation of the effect of a large number of turns in such a machine.

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Title of Project: Electromagnetic Fields in Cavities and Magnets

Person in Charge: R. Gluckstern

Scientific and Professional Staff: A. Dragt, R. Gluckstern, F. Neri, E. Forest, L. Healy, E. Opp, and R. Ryne

Scope of Work

Numerical codes like SUPERFISH, ULTRAFISH, and URMEL are now being used to obtain frequencies of azimuthally symmetric and azimuthally asymmetric modes in electromagnetic cavities. Techniques are now being developed, including finite element methods, to obtain substantial

UNIVERSITY OF MARYLAND
College Park, Maryland

improvement in accuracy. In addition, the cavity impedance obtained from such codes can be related to the determination of beam stability in circular ring and colliding ring applications.

Rare Earth Cobalt (REC) materials are now being widely used for high field permanent magnets. Combinations of REC and iron are being analyzed to learn about saturation limitations in their design.

Explicit solutions for bunched beams interacting with transverse cavity modes in linacs have been developed and are being applied to circular rings and colliding rings in the expectation that one will be able to understand beam stability questions better.

Goals and/or Major Results to Date

Improvements have been made in the accuracy with which cavity frequencies are calculated by the computer code SUPERFISH. Further improvements in both SUPERFISH and ULTRAFISH, a second computer code, appear to be possible, including applications to impedance calculations relevant to beam stability in storage rings. In addition, progress has been made in the design of Rare Earth Cobalt (REC) magnets, including applications involving the combination of REC and iron. Finally, advances have been made in the understanding of beam stability in both linear and circular machines.

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UNIVERSITY OF MASSACHUSETTS
Amherst, Massachusetts

Award No.: DE-AC02-76ER03330

Title of Project: High Energy Physics

Person in Charge: J. B. Shafer

Scientific and Professional Staff: M. Afdal

Scope of Work

The University of Massachusetts Task A group has been completing its analysis of polarized-target data on K^- inelastic reactions, these data having been obtained at the Brookhaven Multiparticle Spectrometer. The experiment was undertaken to demonstrate the utility of their unique target system, a "spin refrigerator", for investigations of multiparticle reactions. Possibilities of future research at electron accelerators are being explored; these include areas of overlap between high energy and nuclear physics.

Goals and/or Major Results to Date

Analysis of the polarized-target experiment has included the identification of $K^-p \to \Lambda\pi^0$ and $K^-p \to Y^*(1385)\pi \to \Lambda\pi^+\pi^-$ events involving polarized protons, with suppression of similar reactions on unpolarized protons in heavy nuclei. The careful event reconstruction and kinematic fitting needed to select polarized-proton data, and to eliminate $\overline{K}^0$ final states, have been achieved. Analysis of the production and decay amplitudes for polarized and unpolarized data is expected to demonstrate the richness of the former and to yield information useful for quark models. Pattern-recognition and Monte-Carlo techniques (for the Brookhaven MPS) have been significantly improved.

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Title of Project: Task B - PEP-4/TPC Collaboration

Person in Charge: R. R. Kofler

Scientific and Professional Staff: R. R. Kofler

Scope of Work

The PEP (TPC) project utilizes a sophisticated particle detecting-identifying apparatus currently installed at the positron-electron collider (PEP) at the Stanford Linear Accelerator Center (SLAC). The central detector of the apparatus is a large drift chamber, the Time Projection Chamber (TPC), which identifies charged particles by the simultaneous precision measurements of particle momentum and ionization energy loss. The apparatus also includes a muon identifying system and electromagnetic calorimeters for the identification of electrons, gamma rays, and the reconstruction of pi zero mesons. After a highly successful data taking run during 1983, the apparatus has been removed from its interaction region at PEP for the implementation of an improvement program including the installation of a "gating" grid on the TPC and a superconducting magnet. These improvements are expected to enhance the momentum resolution of the detector by an order of magnitude. Reinstallation in the collider is expected late in 1984 and the collaboration expects to take data at PEP for the following two to three years.

Goals and/or Major Results to Date

The primary physics goals include: searches for new particles, tests of the standard QCD models through the study of "jet" behavior in positron electron annihilation into quark antiquark pairs (with or without gluon), and the study of reactions resulting from positron-electron annihilations into two photons. Major results obtained so far from the 1983 data sample include precision measurement of production cross sections for most of the known particles (e, mu, pi, K, proton, lambda, Xi, and phi), studies of charge and strangeness correlations within jets, searches for primary quarks and diquarks, and preliminary results from searches for some expected new particles. The most tantalizing recent result is the evidence for a new resonance, a charmed heavy meson, the F*, which decays radiatively into an F meson. The collaboration looks forward to an extensive period of data taking, during which time its performance will be unmatched by any other detector studying positron-electron annihilation at energies between 15 and 30 GeV.

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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts

Award No.: FG02-84ER40164

Title of Project: Modern Geometric Methods in Particle Physics

Person in Charge: I.M. Singer

Scientific and Professional Staff: E. Baum and I. M. Singer

Scope of Work

In recent years it has been widely recognized that gauge theories in elementary particle physics involve fibre bundles in global geometry. As a result, a new liaison between geometry and high energy theoretical physics is being forged. They propose to try and solve some of the major problems in Quantum Field Theory as well as to apply modern mathematical geometric methods to less ambitious questions raised by gauge theories.

They will encourage research which combines both mathematics and physics, in a context that will increase contact and understanding between the two fields. At present, the language barrier remains enormous. Physicists do not know what the "state of the art" is in various fields of mathematics, while mathematicians not only do not know what the major problems of Quantum Field Theory are, but do not enjoy the physical intuition that prompts them and suggests their solution. Sustained contact is in order and one can expect it will bear fruit, as the recent successes indicate.

Both long-term and short-term visitors stimulate the program. Many scientists visiting the group are interested in this research area; and are being invited to the seminar and are spending a day or two talking and working with faculty and students. They feel research in both the mathematics and physics departments are enhanced by the program.

Goals and/or Major Results to Date

Interesting results have been discovered by the application of index theorems to anomalies and through path integral study of the consequences of a cosmological constant.

Index theorems show that nonabelian chiral anomalies are topological in origin. Minimization of the Euclidean action for a scalar field coupled to classical gravity forces the effective cosmological constant to zero.

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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, Massachusetts

Award No.: DE-AC02-83ER40121

Title of Project: Acoustic Emission Technology

Person in Charge: Y. Iwasa

Scientific and Professional Staff: Y. Iwasa, O. Ige, D. Cultice, and L. Thompson

Scope of Work

The project's principal objective is to make acoustic emission technology an integral component of diagnostic techniques for high performance superconducting dipoles and quadrupoles required for high energy physics accelerators. The project's Phase 1 focuses on the development of real-time display instrumentation for acoustic emission signals originating from dipoles. In Phase 2, parallel to further instrumentation development, emphasis will also be placed on correlating acoustic data to dissipation, particularly of mechanical origins, in the magnets: location, sources and mechanisms, energy spectrum. They believe a thorough understanding of the nature of mechanical dissipation within the superconducting magnet winding and its dependence on magnet design parameters is indispensable in achieving design goals in the high-performance dipoles and quadrupoles.

Goals and/or Major Results to Date

A test superconducting dipole magnet operated by Dr. McInturff of Fermi National Accelerator Laboratory in the summer of 1984 was instrumented with AE sensors prepared at MIT and a large set of AE data was collected successfully using equipment designed and built at MIT. Preliminary analysis of data indicates that: (1) the cause of all the premature quenches was conductor motion; (2) premature-quench inducing motion events all occurred at the ends and middle section of the dipole; (3) for each sweep sequence there were approximately one thousand prequench conductor motion events detected, which though not directly responsible for the quenches nevertheless dissipated mechanical energy inside the winding.

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MATHEMATICAL SCIENCES NORTHWEST, INC.
Bellevue, WA

Award No.: DE-AC06-83ER40128

Title of Project: Laser Technologies for Laser Accelerators

Persons in Charge: D. Lowenthal and J. Slater

Scientific and Professional Staff: J. Eggleston, M. Kushner, D. Lowenthal, J. Slater, and R. Taussig

Scope of Work

It has been recognized for some time that the high electric fields near the focus of a powerful laser beam offer the potential of much higher acceleration gradients than are possible with conventional accelerators. These high gradients may provide the best approach to generation of TeV-class particle beams for high energy basic physics experiments. Enthusiasm for the laser accelerator concept has grown significantly during the last several years with the development of a wide range of accelerator mechanisms (i.e., Inverse Free Electron Laser, Inverse Cherenkov, beatwave and grating linac). However, the optical system (laser and optical beam transport) has not received the same scrutiny as the acceleration physics. The scope of this work is to do a comprehensive feasibility study of laser accelerators from the standpoint of the laser optical requirements. The output of this work will be the assessment of current laser technology as it relates to the goals of high energy accelerators.

Goals and/or Major Results to Date

The basic laser accelerator mechanisms have been reviewed from the point of view of laser requirements. In addition, the expected accelerator luminosity requirements have been used to develop tradeoff maps for laser parameters such a pulse length, energy per pulse, and repetition rate. Current goals include completing a survey of existing laser technology and determining optimum matching between laser systems and accelerator mechanisms. Benchmark designs for 50 GeV and 1 TeV accelerators shall be completed as well as recommendations for laser research and development that brings the laser technology into the regime of accelerator requirements.

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UNIVERSITY OF MICHIGAN
Ann Arbor, Michigan

Award No.: DE-AC02-76ER01112

Title of Project: Experimental Particle Physics--Proton Decay

Persons in Charge: D. Sinclair, L. R. Sulak, and J. Vander Velde

Scientific and Professional Staff: J. Allen, D. Casper, C. Chrysicopoulou, R. Claus, S. Errede, G. W. Foster, D. Higby, M. Ikeda, K. Mullen, H. S. Park, S. Seidel, E. Shumard, D. Sinclair, J. Stone, L. R. Sulak, and J. Vander Velde

Scope of Work

Tasks B, F, and M have historically pursued experimental studies in neutrino physics using large, highly instrumented calorimetric detectors and bubble chambers. The present effort involves the search for nucleon decay at the Irvine-Michigan-Brookhaven proton-decay detector near Painesville, Ohio. An 8,000 ton ring-imaging, water Cherenkov calorimeter totally contains atmospheric neutrino events which occur at the rate of one per day. For proton decays into the minimal SU5 model of $e^+\pi^0$, the detector should be sensitive to a lifetime/branching ratio of 10^{33} years. At that level, the neutrino events begin to mimic nucleon decay. For proton-decay modes suggested by supersymmetric and supergravity theories, the anticipated sensitivity is 1 to 3 x 10^{31} years. The detector is currently being upgraded to enhance the light collection by a factor of four. This will improve the discrimination against neutrino events for these models by perhaps an order of magnitude.

The IMB detector is the largest in area, volume, and information content to be built underground. It can study atmospheric neutrinos, search for neutrino oscillations with the baseline of the earth's diameter, and search for point sources of extraterrestrial neutrinos. Monopoles that might traverse the detector and catalyze proton decay would also be detectable.

The specific responsibilities of Michigan in the IMB collaboration include the custom designed on-line data acquisition electronics, the monitoring and calibration hardware, the on-line software, and much of the off-line analysis software.

Goals and/or Major Results to Date

The current limit of 2×10^{32} years for the $e^+\pi^0$ mode is a factor 2000 above that predicted by the minimal SU5 theory of the grand unification of the weak, electromagnetic, and strong interactions. If all the input data of the calculation is forced to increase the prediction, 40 events are expected. They see no candidates for this mode. Apparently nature respects some other unifying theory.

For a host of other nucleon decay modes (e.g., νK^+, e^+K^0, μ^+K^0, νK^0, etc.) the current limits lie at the 1 to 3 x 10^{31} year level.

UNIVERSITY OF MICHIGAN
Ann Arbor, Michigan

Typically for each mode a few nucleon decay candidates exist at the level expected for neutrino-induced background. With the upgrade that will be complete by the end of 1985, the invariant mass of an intermediate heavy decay product (ρ, ω, K^0, η) will be reconstructable, allowing them to reduce the background significantly.

Hundreds of neutrino events have been recorded in the device. Limits on neutrino oscillations, on point sources of neutrinos, and on the flux of proton decay catalyzing monopoles have been set.

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Title of Project: Experimental Particle Physics--High Resolution Spectrometer

Person in Charge: R. P. Thun

Scientific and Professional Staff: C. W. Akerlof, J. W. Chapman, D. I. Meyer, R. P. Thun, D. Nitz, A. Seidl, T. Trinko, and M. Willutzky.

Scope of Work

The primary research activity of this task is a general study of electron-positron annihilations at the Stanford Linear Accelerator Center (SLAC). Since 1977 this group has been a major component of the HRS collaboration working at PEP. HRS is a high resolution spectrometer which is expected to accumulate data at least through 1985. By that time, they expect to have made a major contribution to the understanding of heavy quark production in 29 GeV e^+e^- annihilations. They have already observed very clean signals of charmed quark production in a number of different channels. They are also pursuing an analysis of higher-order QED interactions and a search for new heavy neutral particles.

In the future, they are planning to continue their research in electron-positron physics at higher energies at the SLAC Linear Collider (SLC). They have, therefore, joined the MKII/SLC collaboration and intend to make two major contributions to this experiment. One of these is a research and development project which will hopefully lead to the implementation of a very high precision particle tracker based on the technology of CCD's (charged-coupled devices). Such a tracker will permit a detailed study of events with vertices from charm, beauty, or tau decay. The other contribution is the construction of tracking and calorimetric detectors to be placed at very small angles to the SLC beams. Such detectors are essential for the determination of the SLC luminosity and the rejection of backgrounds in measurements of $e^+e^- \to \gamma\nu\bar{\nu}$. The physics program of SLC is expected to begin in 1987.

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UNIVERSITY OF MICHIGAN
Ann Arbor, Michigan

Title of Project: Counter Group

Person in Charge: A. D. Krisch

Scientific and Professional Staff: A. D. Krisch, K. M. Terwilliger, D. G. Crabb, A. M. T. Lin, R. Raymond, and P. Cameron

Scope of Work

This group is studying proton-proton spin physics, especially high momentum transfer elastic scattering. They are also very involved in the technical developments necessary to carry out these experiments, including modifying the ZGS for the acceleration of polarized protons and polarized proton target and polarized gas jet development. Starting in 1970, they took a major role in conceiving and implementing the acceleration of the world's first high energy polarized proton beam at the Argonne ZGS. By 1979, the final year of ZGS operations, they had successfully completed their program of measuring the spin-spin pp elastic cross sections at 6 and 12 GeV/c, and at 90°cm over the full ZGS momenta range of 2 to 13 GeV/c. They found that the ratio of the (transverse) spin-parallel to spin-antiparallel cross sections $[d\sigma/dt_{\uparrow\uparrow}:d\sigma/dt_{\uparrow\downarrow}]$ increased dramatically, to a value of about 4 at $P_{\perp}^{2} = 5\ (GeV/c)^{2}$ with the $P_{\perp}^{2}$ dependence of the fixed-angle 90°cm spin experiment almost identical to the $P_{\perp}$ dependence in the 12 GeV/c fixed-energy spin experiment. These results were not predicted by standard QCD theory. To extend this research to higher energies they initiated studies at the 1977 "Ann Arbor Workshop" and have since been involved in developing a polarized proton capability at the Brookhaven AGS; they built the 12 pulsed quadrupole magnets to preserve the proton polarization by resonance jumping, and are responsible for the internal and high energy polarimeters. One of them has overall responsibility for the Polarized Beam Commissioning, which has recently had some success.

Goals and/or Major Results to Date

They are presently aiding the AGS staff in commissioning the accelerated polarized proton beam. Their first experiment with this beam which will study the high energy behavior of the spin-parallel to anti-parallel cross-section ratio, is scheduled for summer 1984. They are also measuring th single spin asymmetry parameter, A, with the unpolarized beam and their high-cooling power polarized proton target at the AGS. They have completed one set of measurements, out to $P_{\perp}^{2} = 6\ (GeV/c)^{2}$ at 28 GeV/c [illegible] observed a totally unexpected large positive value of A at their highest $P_{\perp}^{2}$; they plan to extend these measurements to even higher $P_{\perp}^{2}$.

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UNIVERSITY OF MICHIGAN
Ann Arbor, Michigan

Title of Project: Theory

Persons in Charge: M. B. Einhorn and Y.-P. Yao

Scientific and Professional Staff: M. B. Einhorn, G. L. Kane, Y. Tomozawa, M. Veltman, D. Williams, Y.-P. Yao, V. Baluni, M. Duncan, A. Hasanfratz, J.-M. Frere, R. Philippe, and T. Sterling

Scope of Work

This theoretical group pursues research on the frontier of elementary particle physics. Presently, their primary focus is on (1) standard model predictions for physics in the hundreds of GeV energy range, and (2) what lies beyond the standard model. Lately, they have not emphasized research on the lattice approach to gauge theories or on perturbative QCD, although members of this group have worked in these areas in the past and continue to follow results.

In addition, they have considerable interaction with their experimental colleagues at Michigan and elsewhere. Individuals in this group also contribute to the national program through their participation on the planning advisory committees of Fermilab and Brookhaven National Laboratory and on HEPAP. During the past year, members have also attended several workshops dealing with physics possibilities at the SSC.

Finally, during June 1984, they hosted and directed the Theoretical Advanced Study Institute for advanced graduate students in high energy physics, sponsored jointly by DOE, NSF, and the University of Michigan.

Goals and/or Major Results to Date

During the past year, members of this group published papers on supersymmetric extensions of the standard model and their experimental implications at energies observable now or at the next generation of accelerators, on model building in a new class of finite field theories, on effects to be anticipated for a heavy Higgs boson in the standard model, on possible theoretical mechanisms to account for the "anomalous" radiative events observed at the CERN $S\bar{p}pS$, on composite models of the Higgs boson and the origins of mass, the interpretation of high energy cosmic rays, and possible improvements on limits on the galactic monopole flux.

These topics are all at the limits of current understanding of the fundamental laws of nature and will no doubt continue to characterize the direction of their research.

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UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota

Award No.: DE-AC02-83ER40105

Title of Project: Theoretical High Energy Physics

Person in Charge: S. Gasiorowicz

Scientific and Professional Staff: S. Gasiorowicz, D. Geffen, H. Suura, T. Walsh, S. Rudaz, D. Reiss, V. Visnjic, J. Johnson, W. Berglund, M. Hanck, M. Nicolic, T. Kurai, X. Q. Li, and I. Sarcevic

Scope of Work

The High Energy Theory group is engaged in the following tasks: (1) the clarification of the phenomenological implications of QCD, including the low energy spectrum and hadronization; (2) the phenomenological implications of grand unified theories, supersymmetric and supergravity theories, and a search for signals of new mass scales; (3) the detailed working out of the consequences of the Standard Model; and (4) the interplay of cosmology and particle physics. In all cases, the thrust is towards understanding the currently accepted theories of the interactions and to searching for evidence for a substructure to the Standard Model.

Goals and/or Major Results to Date

Members of the High Energy Physics group have made contributions in the following areas: the study of the mass matrix in unified theories and the impact on decay modes of the proton, monopole catalysis, variational wave functions in QCD, asymptotics in two-point functions and trajectories in confined systems, radiative decays of hyperons, and symmetry breaking in supersymmetric grand unified theories.

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UNIVERSITY OF MINNESOTA
Minneapolis, Minnesota

Title of Project: Experimental High Energy Physics

Persons in Charge: H. Courant, K. Heller, M. L. Marshak, E. A. Peterson, K. Ruddick, and M. Shupe

Scientific and Professional Staff: T. Joyce, P. Lukens, S. Heppelmann, B. Baller, R. Benson, G. Blazey, N. Grossman, S. Heilig, C. James, M. Lau, K. Thorne, D. Wahl, S. Werkema, S. Saroff, D. Rosen, and U. DasGupta

Scope of Work

Work on this project includes experimental investigations of the strong and electromagnetic interactions by means of particle scattering experiments and tests of grand unified and supersymmetric models through a search for proton decay. An ancillary topic is a study of astrophysical phenomena through measurement of deep underground cosmic ray muons using the proton decay apparatus.

The particular topics under current investigation are: (1) a measurement of the properties of direct production of photons at large transverse momentum in very high energy collisions (at Fermilab); (2) a search for proton decay and a study of cosmic ray phenomena (University of Minnesota laboratory at Soudan, MN); (3) a study of quantum chromodynamics through measurement of cross-sections and polarizations at large transverse momentum for a number of exclusive strong interaction processes (at Brookhaven); and (4) a precision measurement of the CP violation parameters on neutral kaon decay.

Goals and/or Major Results to Date

Major results to date include: (1) a lower limit on the proton lifetime; (2) an upper limit on the flux of magnetic monopoles; (3) anomalous time and angle correlations of cosmic ray multimuon events; (4) evidence for direct photon production with incident pions and protons; (5) precision measurement of hyperon magnetic moments; (6) measurement of the electromagnetic couplings of several vector and tensor mesons; and (7) cross-section and polarization measurements for large angle rho production in pion-proton collisions.

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MOUNT HOLYOKE COLLEGE
South Hadley, Massachusetts

Award No.: DE-AC02-78ER04831

Title of Project: Search for Neutrinoless Double Beta Decay in Molybdenum 100

Person in Charge: H. W. Nicholson

Scientific and Professional Staff: H. Nicholson and M. Deady

Scope of Work

The project involves the development of large area, high purity, silicon solid state detectors which will be interleaved with thin sheets of isotopically pure molybdenum 100 to look for neutrinoless double beta decay with high sensitivity. The experiment is expected to be capable of measuring neutrino decay lifetimes less than or of the order of 10^{23} years in molybdenum 100.

Goals and/or Major Results to Date

Progress has been made in measuring and improving the qualities of the silicon oxide required to fabricate high purity silicon detectors. Silicon, silicon oxide interface trap densities have been reduced by two orders of magnitude. A prototype detector array has been built and tested using four lithium drift silicon detectors and is producing results consistent with background estimates at sea level.

Their present goal is to build approximately 10 percent of the complete detector array with large area, thin window, lithium drift silicon detectors and begin taking data while the high purity detector development is under way.

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NATIONAL BUREAU OF STANDARDS
Gaithersburg, Maryland

Award No.: DE-AT01-79ER10426

Title of Project: A New Determination of the Fine-Structure Constant; also a Study of Fractional Charge Electrometers.

Person in Charge: E. R. Williams

Scientific and Professional Staff: G. R. Jones, Jr., P. T. Olsen W. D. Phillips, and E. R. Williams

Scope of Work

The objective of this project is to obtain a value for the fine-structure constant, α, which is both independent of quantum electrodynamic (QED) theory and accurate to 1-2 parts in 10^8. Such a value will enable the critical comparison of experimentally determined values of QED-dependent quantities such as the anomalous magnetic moment of the electron with their QED theoretically calculated values. In actual fact, α will be obtained by measuring the gyromagnetic ratio of the proton, γ_p, to an accuracy of 2-4 parts in 10^8 and then combining this result with the numerical values of already well-known fundamental physical constants such as the speed of light and the Rydberg constant. The success of the experiment depends critically on the accuracy with which the dimensions of a single-layer precision solenoid wound on a fused silica form may be determined, as well as the accuracy with which the NBS as-maintained electrical units (volt via the Josephson effect and ohm via the Thompson-Lampard calculable capacitor) can be realized in the NBS nonmagnetic laboratory where the experiment is being carried out. New apparatus must be constructed and new techniques developed including a precision solenoid 2.2 m long and a completely automated system which includes a multi-axis laser interferometer for making the dimensional measurements. They are working closely with the quantum Hall experiment in progress in the same division. That experiment combined with this effort will provide the most accurate value of α.

In their investigations for alternate methods to measure α, they have come up with a novel method to detect electric charge. They plan to apply this technique to an experiment designed to search for and investigate fractionally charged matter.

Goals and/or Major Results to Date

Just prior to the initiation of this project, a determination of γ_p accurate to 2 in 10^7 was completed resulting in a value of α accurate to 1 in 10^7 [Phys. Rev. Lett. 42, 1575 (1979)]. Based on the experience gained during the course of that work, the one part in 10^8 version of the experiment is under construction. A fused silica form for the most critical element of the new determination, the 2.2 m precision solenoid, has been constructed with μm precision using grinding and precision lapping techniques. The solenoid and measurement system are

NATIONAL BUREAU OF STANDARDS
Gaithersburg, Maryland

now operational and they have a resolution of 0.02 µm for the pitch and radial variations of the solenoid. Their present accuracy for these dimensional measurements is 0.1 µm (0.1 ppm). The tedious task of evaluating the uncertainties and improving the measurement is in progress.

A fractional charge electrometer based on an earlier design [E. R. Williams and G. T. Gillies, Lett. Nuovo Cimento 37, 520 (1983)] has been fabricated. They are assembling the system now but will not have any indication of its usefulness in detecting fractional charges until they get it running.

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1055

NATIONAL BUREAU OF STANDARDS
Boulder, Colorado

Award No.: DE-AI01-79ER10354

Title of Project: Development of Standards for Superconductors

Persons in Charge: A. F. Clark and L. F. Goodrich

Scientific and Professional Staff: E. S. Pittman

Scope of Work

The ultimate goal of this research program is to develop fundamental understanding, consensus standard definitions, consensus standards of measure, and standard reference materials for superconductor parameters.

The key parameters in the commerce of superconductors need standard definitions and standards of measure. These parameters include: critical current, stability, strain dependence, transient loss, critical magnetic field, and critical temperature. They are conducting research on superconductor paremeter measurement practices and problems in support of the creation of these standards. The present research is focussed on critical current measurements on large conductors (600 to 6000 A).

Goals and/or Major Results to Date

They coordinated the formation of an American Society for Testing and Materials (ASTM) subcommittee on Superconductors B01.08 as a forum for consensus standards. A standard definition of terms for superconductivity and a standard test method for the measurement of critical current were adopted by ASTM. The first standard reference material (SRM) for the determination of critical current was characterized and made available for purchase. They have more than 30 publications presenting research results to the superconductor community.

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NAVAL RESEARCH LABORATORY
Washington, DC

Award No.: DE-AI05-83ER40112

Title of Project: Theoretical and Computational Research in the Focused Transport of Charged Particle Beams

Person in Charge: I. Haber

Scientific and Professional Staff: H. Dantsker, I. Haber, and M. Reiser

Scope of Work

Research is directed toward understanding the growth of beam emittance and the related limits on phase space density during focused transport and bunching. Since emittance growth, especially when the self-consistent electric forces are included, can be a highly nonlinear process, computer simulations play a major part in this research. The parameter regime to be studied has been chosen both for general applicability and also for comparison with the behavior of the low emittance transport experiment at the University of Maryland.

Goals and/or Major Results to Date

Simulations to date have indicated that the nonlinear behavior depends more strongly on focusing geometry than would be expected from the linear theory. Saturation of the nonlinear evolution has been found to result in negligible rms emittance growth in a number of instances.

Current goals call for a more direct comparison of the details of numerical simulation to experimental data, as well as an expansion of beam dynamics in both simulation and experiment to include bunching.

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Award No.: DE-AI05-83ER40117

Title of Project: High Energy Laser Driven Accelerators (Theory)

Persons in Charge: P. Sprangle and C. M. Tang

Scientific and Professional Staff: Y. Y. Lau, W. Marable, and H. Freund

Scope of Work

Laser driven particle accelerating schemes are currently receiving considerable attention. Existing types of synchrotron and linear accelerators are nearing their economic limits in going much beyond a few TeV in energies. The availability of high power laser beams ($>10^{14}$ watts) with electric fields as high as 10^9 V/cm brings about the possibility of using these high fields to accelerate particles. Direct use of these fields for continuous particle acceleration is not possible due to the transferse polarization and rapid oscillation of the fields.

Goals and/or Major Results to Date

For the IFEL accelerator schemes, NRL proposed the self-consistent tapering of the wiggler period as well as the amplitude of the magnetic wiggler fields. The development of a self-consistent analysis including radiation depletion and space charge effects has been carried out.

For the LBWA schemes, NRL has analyzed the excitation of the plasma waves by two laser beams, whose frequency difference is approximately the plasma frequency. The nonlinear analysis is fully relativistic and includes mismatching of the laser beat frequency to the plasma frequency, time dependent laser amplitudes, and an applied transverse magnetic field (surfatron).

The research goal for FY 1985 is to self-consistently analyze the various stimulated nonlinear instabilities associated with the injection of two intense laser beams into a plasma in the LBWA.

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UNIVERSITY OF NEW MEXICO
Albuquerque, New Mexico

Award No.: DE-FG04-84ER40166

Title of Project: Dynamics of Fields and Particles

Person in Charge: K. Cahill

Scientific and Professional Staff: K. Cahill

Scope of Work

K. Cahill carries out basic research in high energy theoretical physics. The subject of the research is the description of the four fundamental interactions by means of gauge theory. The methods used include Monte Carlo simulations of path integrals on supercomputers. One graduate student, Randolph Reeder, and one postdoctoral fellow, Sudhakar Prasad, (neither supported by DOE), collaborate in this research.

Goals and/or Major Results to Date

The goals of this project are the development of theoretical concepts and numerical methods in gauge theories of particle interactions. This research is worthwhile because it may lead to a better understanding of the basic structure of matter.

During the first three years of DOE funding, Cahill introduced a new way of unifying gravity with the strong and electroweak interactions and made other contributions to the gauge theory of noncompact groups. He also developed and tested new computerized techniques for approximating path integrals. These techniques can be used to calculate physical quantities that are inaccessible by perturbation theory.

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CITY UNIVERSITY OF NEW YORK
New York, New York

Award No.: DE-AC02-83ER40107

Title of Project: Experimental Investigation of the Production of Glueballs and Meson Resonant States

Person in Charge: S. J. Lindenbaum

Scientific and Professional Staff: C. S. Chan, J. Goo, M. A. Kramer, S. J. Lindenbaum, and J. Piekarz

Scope of Work

The group's research activities include two major areas of basic investigation in strong interaction physics.

1. The study of glueball production in the Zweig forbidden process $\pi^- p \rightarrow \phi\phi n$ at 22 GeV/c. The Zweig diagram describing this process is disconnected and thus is expected to strongly filter out conventional mesonic states from contributing to the $\phi\phi$ system. However, if a glueball with positive charge conjugation exists within the mass range 2-3 GeV it is expected to break down the Zweig suppression and be seen in the $\phi\phi$ system. Three generations of experiments starting in 1978 with 100 events and obtaining $\approx$ 4,000 events by mid-1983 have been performed with the BNL MPS II Spectrometer by a BNL/CCNY collaboration.

2. A search for glueball and other meson resonant states is being made in the reactions

$$\pi^- p \rightarrow K_S^0 K_S^0 \pi^0 n$$

$$K_S^0 K_S^0 \eta^0 n$$

$$K_S^0 K_S^0 n.$$

A Brandeis/BNL/CCNY/Duke/Notre Dame collaboration is in the process of running this experiment with MPS II at BNL.

Goals and/or Major Results to Date

1. The three new states found in $\pi^- p \rightarrow \phi\phi n$, namely the [$g_T(2120)$, $\Gamma \approx 300$, $g_T(2220)$, $\Gamma \approx 200$, $g_T(2360)$, $\Gamma \approx 150$ in MeV units] are concluded to be produced by glueball(s) if one assumes the following two simple axioms which merely represent modern QCD practice: a) QCD is correct; b) The OZI rule (i.e. Zweig suppression) is universal for weakly coupled glue in Zweig disconnected diagrams where the disconnection is due to the creation or annihilation of new quark flavors.

2. The goals of this experiment are to search for possible glueball states decaying into $K_S^0 K_S^0 \pi^0$, $K_S^0 K_S^0 \eta^0$ and $K_S^0 K_S^0$. They also will investigate the other meson resonance states in these reactions.

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CITY UNIVERSITY OF NEW YORK
New York, New York

Title of Project: Development of an Electronic Fine Sampling Ionization Loss Particle Identifier Using a Longitudinal Drift Chamber

Person in Charge: S. J. Lindenbaum

Scientific and Professional Staff: C. S. Chan, J. Goo, M. A. Kramer, J. Lindenbaum, and J. Piekarz

Scope of Work

A BNL/CCNY collaboration has previously demonstrated with a longitudinal drift chamber, that electronic five track segment sampling can increase the selectivity for particle identification via ionization loss. This chamber was a one-layer 4" x 4" chamber and the increase in selectivity obtained was a factor of two. The present program is to test this new method in a multi-layer chamber using the reliable and inexpensive MPS II drift chamber technology. In previous tests with a multi-layer chamber, it was found that corrections for baseline shifts had to be made in order to maintain the increased sensitivity. A three layer chamber with capability of simulating various geometries (including screens) is now being tested at the AGS. This chamber uses MPS II technology and, therefore, should be both reliable and economical.

Goals and/or Major Results to Date

The next objective is to obtain the increased sensitivity with this new MPS II technology longitudinal drift chamber. The eventual goal is to develop an MPS II chamber size ionization loss particle identifier for use with glueball production and other MPS II experiments. This is expected to enhance the glueball research and other MPS II programs as well as serve as a practical demonstration of the technique so that wide scale use by the physics community can follow.

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1061

STATE UNIVERSITY OF NEW YORK AT ALBANY
Albany, New York

Award No.: DE-AC02-78ER05001

Title of Project: Experimental High Energy Physics and Applications of Channeling

Persons in Charge: C. R. Sun and W. M. Gibson

Scientific and Professional Staff: M. S. Alam, Z. H. Bian, I. J. Kim, F. P. Sun, W. Li, M. Pisharody, V. Tanikella, and R. Wijayawardana

Scope of Work

SUNY has been working on the channeling of high energy particles through single crystals, aiming at possible applications to particle physics experiments and/or accelerator beam transport. Over the past few years they have conducted experiments at Fermilab, SLAC, Dubna, and Serpukhov. The topics of study included fundamental properties of channeling of GeV particles through single crystals of silicon and germanium; channeling radiation from GeV positrons; and the steering of charged particles by bent single crystals. They concentrated their effort in areas where application to particle physics experiments and beam transport systems appeared most favorable.

Most recently, with the addition of Professor M.S. Alam to their faculty, they are starting a new activity at Cornell on the B-meson physics and the upgrading of the CLEO II detector. In the meantime, they will continue their work on channeling.

Goals and/or Major Results to Date

They have succeeded in steering high energy particles through bent single crystals (Si). Most recently, they have accomplished one of their goals in replacing an existing magnetic dipole pair in a secondary beam line (M-bottom, Fermilab) with a bent single silicon crystal. This crystal septum bends beams up to 400 GeV. They have observed channeling radiation from GeV positrons. Their goal is to use this radiation for mass tagging at super high energies. Other goals include charmed particle lifetime and charmed particle magnetic moment measurements using bent crystals. At Cornell, they will work on B-meson physics and upgrading of the CLEO II detector.

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1062

STATE UNIVERSITY OF NEW YORK
Binghamton, New York

Award No.: DE-AC02-83ER40108

Title of Project: Theoretical High Energy and Nuclear Physics

Person in Charge: C. A. Nelson

Scientific and Professional Staff: C. A. Nelson

Scope of Work

This work is in the area of theoretical high energy and nuclear physics. Motivated by the fact that the non-cancellation of the infrared divergences in quantum chromodynamics can be avoided by using soft degenerate states or coherent states in the initial state, they are investigating the possible effects of introducing these degenerate states on the q_T dependence of the one-loop finite piece in hard scattering subprocesses like $q\bar{q}\to\gamma^*X$ in the Drell-Yan process. They are using Kinoshita diagram identities, a summation over spectator interactions, and Ward identities to establish whether the on-shell Glauher region is a gauge invariant concept which can be physically isolated and whether there are, indeed, k_T fluctuations and color-correlation effects. They also are examining whether the usage of a quark-gluon degenerate state basis will maintain (or modify) the simple property of factorization of QCD processes into short-distance and long-distance parts. Motivated by the large second order π^2 type terms and large soft gluon corrections in some hard processes, they are using gauge invariance to develop a systematic method for factorization and resummation of these large infrared effects.

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1063

STATE UNIVERSITY OF NEW YORK
Stony Brook, New York

Award No.: DE-AC02-80ER10699

Title of Project: Experimental High Energy Physics Research Using Electromagnetic Energy Calorimetry

Person in Charge: M. Marx

Scientific and Professional Staff: M. Marx, D. Hedin, and L. Godfrey

Scope of Work

This group has had three main lines of research--low-energy neutrino physics, detector development, and high energy hadron collider experiments.

The group has been involved in an experiment at Brookhaven to study the elastic scattering of neutrinos and antineutrinos from electrons and protons. The group has contributed two major elements of the detector--a 30-ton shower detector and a muon spectrometer and is involved in the analysis of the neutrino proton data.

Research has been performed using low-cost, highly segmented arrays of lead glass as prototypes for hadron collider experiments. Studies of radiation damage to lead glass have also been performed.

Work is in progress on the design and development of an experiment approved for the D-Zero area at the Fermilab 2 TeV $\bar{p}p$ Collider. This experiment will stress the measurement of leptons and hadron jets over most of the solid angle.

Goals and/or Major Results to Date

The group has recently published first results on the $\nu_\mu e$ elastic scattering which indicate the power of the experiment. By summer 1984 they will report both $\nu_\mu e$ and $\bar{\nu}_\mu e$ results leading to one of the most sensitive measures of $\sin^2\theta_W$. They will also have first results on $\nu_\mu p$ and $\bar{\nu}_\mu p$ scattering.

They have published reports of the utility of low-cost lead glass and the use of a highly-segmented array for discriminating between electrons and hadrons. They will also soon report on the use of doped lead glass which is more resistant to radiation damage.

The group is involved in the construction of a major new detector for the D-Zero region at Fermilab which will study 2 TeV $\bar{p}p$ collisions.

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1064

UNIVERSITY OF NORTH CAROLINA
Chapel Hill, North Carolina

Award No.: DE-AS05-79ER10448

Title of Project: Gauge Theories and Unification

Persons in Charge: P. H. Frampton, Y. J. Ng, and H. Van Dam

Scientific and Professional Staff: P. Moxhay, Y. J. Ng, H. Van Dam, K. Yamamoto, and P. H. Frampton

Scope of Work

The group pursues research in elementary particle theory. All members are active in work on one or more of the topics: QCD and grand unification, supergravity and Kaluza-Klein theory, general relativity, and cosmology.

There are frequent visitors from the eastern United States who give seminars and sometimes participate in the ongoing research program. Also, participants in the program often travel to conferences and other research centers.

Goals and/or Major Results to Date

Members of this group have recently made important contributions to: perturbative QCD and quarkonia; global supersymmetry as applied to grand unification and to composite models; approaches to family unification; higher dimensional theories especially their chiral anomalies, etc.

Their goal is to maintain an interesting and active program in particle theory research.

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1065

NORTHEASTERN UNIVERSITY
Boston, Massachusetts

Award No.: DE-AC02-82ER40059

Title of Project: Gauge Theories and Unification of Elementary Particle Interactions

Person in Charge: M. T. Vaughn

Scientific and Professional Staff: M. T. Vaughn

Scope of Work; Goals and Major Results to Date

The derivation of the two-loop renormalization group equations for the gauge couplings, Yukawa couplings, and scalar quartic couplings in a general renormalizable theory are being completed. Questions of scheme dependence, which are especially relevant to the renormalization group analysis of supersymmetric theories, are also being investigated.

These equations will then be combined with one-loop boundary conditions to study the evolution of effective Lagrangians through various stages of symmetry breaking. Constraints on masses and decay rates due to the presence of infrared fixed points in the equations for the Yukawa and scalar quartic couplings, will also be studied.

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NORTHWESTERN UNIVERSITY
Evanston, Illinois

Award No.: DE-AC02-76ER02289

Title of Project: High Energy Experimental Physics

Person in Charge: J. Rosen

Scientific and Professional Staff: W. Sakumoto, L. Spiegel, C. Winter, and S. Del Champs

Scope of Work

1. Final analysis of Fermilab E-515 is in progress. S. Sontz, L. Crimaldi, and W. Sakumoto have completed theses; C. Winter and S. Delchamps will finish in Spring 1985.

   An article on $\mu^{\pm}e^{\pm}$ correlations and associated charm production has been submitted to Phys. Rev. Lett. Some evidence for $D^0(\overline{D}^0)$ and $F^{\pm}$ production was observed but with limited statistical significance. A portion of the running time was devoted to triggering on large $p_{\perp}$ showers in the liquid argon calorimeter. A study of γ, π^0 and η^0 production is under way. A paper describing design and operation of the E-515 liquid argon calorimeter has been submitted to NIM.

2. The major effort for 1984/1985 involves construction and installation of equipment for E-705/T-721. E-705 features a large aperature multiparticle spectrometer for use in high-intensity $\bar{p}$,p, or π^- beams. The spectrometer includes a high-resolution EM calorimeter consisting of blocks of Pb glass with scintillating glass around the central region.

   Multiple triggers allow study of:

   a. Dimuons: $\bar{p}p \to x+x \to \gamma+4+x \to \gamma+\mu^+\mu^-+x$,

   b. High $p_{\perp}$ direct photon production,

   c. Diphoton production; in this case the superior mass resolution will lead to good π^0 rejection.

T-721 is an extremely innovative and daring effort with potentially dramatic and far-reaching impact. They intend to study the CP-violating decay $K_L \to \pi^+\pi^-$ with one overall-important variation. For the first time the K_L sample will have been generated from a hadronic reaction ($\bar{p}p \to K_L + X$) which is CP symmetric.

Current knowledge of CP violation eminates from the K_L system. Two recent measurements (Fermilab, BNL) suggest that the ratios $\pi^+\pi^-/\pi^0\pi^0$ are the same for K_S and K_L. This is not natural to the currently popular Kobayashi-Maskawa model; it is natural to the older superweak model. They have conjectured that the CP mixing in K_L and K_S decay is somehow initiated in the CP asymmetric environment of the production processes studied to date. This revolutionary viewpoint must be tested experimentally. This will be done with straightforward perturbations in the upstream portion of the E-705 spectrometer.

They are constructing a large P.W.C. module for additional tracking upstream of the manget; in addition, they are installing L.E.D. light flashers on the 600 scintillation counters of the hodoscopes. They have also undertaken the deadening of all P.W.C. modules in the beam region and the design of a flexible support structure for all P.W.C.'s upstream of the large-aperature magnet.

Running for E-705/T-721 will begin January 1985.

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Title of Project: High Energy Experimental Physics

Person in Charge: Donald H. Miller

Scientific and Professional Staff: F. Luehring, C. Guss, and H. Hensley

Scope of Work

1. It is widely agreed that QCD predicts the formation of a quark-gluon plasma at sufficiently high temperature and/or pressure. Anomalous lepton production would be expected with the formation of this new state of matter. They are currently measuring the production of electrons in proton-nucleus and nucleus-nucleus collisions at the LBL Bevalac. The existing two-arm spectrometer (TASS) has been instrumented with scintillator hodoscopes for momentum measurement, and Cerenkov counters and Pb glass for electron identification. Running will be completed in January 1985 and analysis in summer.

2. Lowest-order QCD predicts only small single-spin effects at high energies; nevertheless large polarizations have been observed in Λ production, etc. They are involved in a collaborative program at Fermilab to study spin effects (E-704) systematically in total cross sections, Λ production, and in charged and neutral pion production.

   The incident beam of polarized p's or $\bar{p}$'s is produced by Λ ($\bar{\Lambda}$) decay. In this case the effective source area is large and the polarization of each particle must be deduced from its momentum (200±10 GeV/c) and its transverse position at the intermediate focus. These will be measured on-line with tagging hodoscopes to be constructed in 1985.

They are primarily concerned with the measurement of cross-section differences for parallel and antiparallel helicity states. This requires the addition of a polarized target. If quark-antiquark annihilation into vector mesons is important, the cross-section difference for $\bar{p}p$ will be significantly larger than for pp. Hodoscopes necessary for these measurements will be constructed in 1986; running is scheduled for 1987.

3. With a long lead time for E-704 some effort will be committed to E-705/T-721 with J. Rosen. Construction has been undertaken of 360 PM bases for the Pb-glass wall used in direct photon detection; in addition, construction of the proportional chamber for tracking immediately behind the liquid hydrogen target will be started. Running will begin January 1985.

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Title of Project: Design, Construction, and Testing of Equipment for D-Zero and E-687

Persons in Charge: D. Buchholz and B. Gobbi

Scientific and Professional Staff:

Scope of Work

This task is presently involved in the design, construction and testing of equipment for two experiments at Fermilab: the D-Zero project for TeV I and experiment E-687 to run at TeV II. The physics results expected to be produced by these two projects promise to be numerous and of great scientific interest. B. Gobbi has also taken part in the last run of an experiment at TRIUMF to measure the polarization parameter ξ and the asymmetry parameter ξ of the muon decay. The analysis of the 20 million events collected during this last January run is presently in progress on the VAX at Northwestern.

For the D-Zero project, Northwestern shares the responsibility with SUNY Stony Brook for the central tracking of the detector and specifically for the endcap drift chambers.

For the E687 photoproduction experiment, they are building the muon counters and must also construct the scintillator hodoscopes and the hadron calorimeter.

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Title of Project: High Energy Physics Research

Person in Charge: D. Buchholz and D. Miller

Scientific and Professional Staff: D. Buchholz and D. Miller

NORTHWESTERN UNIVERSITY
Evanston, Illinois

Scope of Work

This task is responsible for the shared resources of the DOE contract. This includes two full-time electronic technicians and the computer resources.

This past year, the work emphasis for the technicians has been for Fermilab E-705, construction of a $p\bar{p}$ beam monitor for the Fermilab TeV I project, and maintaining the computer resources. During this coming year, it is expected that major construction work will occupy most of the technicians' time for E-687, E-705/T-721, and D-Zero.

The VAX 11/780 computer has been used extensively by almost all high energy physicists at Northwestern. It has been used for the following:

1. Analyze ISR experiment R211
2. Analyze Bevalac experiment E-670H
3. Analyze Triumph muon experiment
4. Study the polarized beam for FNAL experiment E-704
5. Monte Carlo FNAL E-710 to understand acceptance
6. Monte Carlo FNAL T-721 to study acceptance
7. Monte Carlo FNAL E-687 to study production models

The proposed technical program includes continuation of a majority of these programs plus additional computation needed for E-705 and the D-Zero project. They also propose to increase their capability in data acquisition and testing with the PDP11/34, in high speed graphics in conjunction with the Northwestern contribution, in networking their laboratory with collaborating laboratories and in improving their hard copy capability.

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NORTHERN ILLINOIS UNIVERSITY
Dekalb, Illinois

Award No.: DE-AC02-78ER05023

Title of Project: High Energy Physics

Person in Charge: F. E. Taylor

Scientific and Professional Staff: F. E. Taylor

Scope of Work

This task is concentrated on a study of high energy neutrino interactions using a 340 metric ton fine grained neutrino detector developed at Fermilab. The emphasis of this program is to probe the small scale structure of the nucleon using the weak neutral current. They reconstruct the kinematics of the neutral current deep inelastic scattering events by measuring the angle of energy flow of the recoil hadron shower and using the incident neutrino energy determined by narrow band neutrino beam. Comparisons are made with the deep inelastic neutrino scattering by the charged current interaction. The data are used to test the current theories of the electroweak interaction and of the structure of the nucleon described by quantum chromodynamics.

Since the detector is fine grained, it has a high pattern recognition capability enabling certain rare neutrino reactions to be studied. Some effort has been spent in studying the feasibility of a high statistics neutrino-electron elastic scattering measurement and searching for neutrino oscillations.

Goals and/or Major Results to Date

They have compared the scaling variable x distribution of the weak neutral current neutrino scattering with that of the charged current neutrino scattering. The findings indicate that the standard model is satisfied. In addition, the total neutrino-nucleon cross section will be determined. They have searched for muon neutrino--heavy neutrino oscillations using energy constraints of quasi-elastic events in the narrow band neutrino beam.

The measurement of the properties of the weak neutral current in neutrino scattering at high energy will be extended into a new energy region with two scheduled experiments using the detector at the Tevatron.

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1071

OHIO STATE UNIVERSITY
Columbus, Ohio

Award No.: DE-AC02-76ER01545

Title of Project: Theoretical Investigations in High Energy Physics

Person in Charge: W. F. Palmer

Scientific and Professional Staff: K. Lane, W. Palmer, S. Pinsky, J. Shigemitsu, K. Tanaka, W. Wada, S.C. Chao, K. Olynyk, and J. McCabe

Scope of Work

Theoretical investigations will be made on a wide range of topics. The unifying theme is the theoretical and phenomenological study of gauge theories.

Work continues on phenomenological issues related to experimental tests of quark and lepton substructure and to the search for Higgs mesons and composite technicons. Production cross sections and estimated backgrounds for the Superconducting Super Collider will be studied.

The study of glueballs in QCD, relating especially to the experimental and theoretical status of $\iota(1400)$ and other states of interest, will be continued. The QCD anomaly terms in chiral effective Lagrangians will be studied.

Work continues on composite models, grand unified theories under supersymmetry, and their possible low-energy manifestations in particle mass spectra. Supersymmetric string theory and dimensional reduction in supergravity will be studied.

Investigations in lattice gauge theory will continue to study non-perturbative structure of gauge theories with emphasis on realization of chiral symmetries. The behavior of gauge theories at finite temperature is also being studied in connection with the phase transitions expected in various early universe scenarios.

Goals and/or Major Results to Date

The main topics of investigation have been theory, construction, and application of gauge models. The major subareas of the research this year are: (1) Realization of fermion chiral symmetries, either through massless composite fermions (exact symmetry) or Goldstone bosons (spontaneously broken symmetry); applications to dynamically broken gauge theories. (2) Chiral symmetry, effective Lagrangians and anomalies. (3) Supersymmetry and grand unified theories. (4) Neutrino mixing in grand unified theories. (5) Implications of the large N limit. (6) Composite models of leptons and quarks; experimental test for quark and lepton substructure. (7) Lattice gauge theories. (8) Glueball theory and phenomenology. (9) Chaos in quantum mechanical systems.

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OHIO STATE UNIVERSITY
Columbus, Ohio

Title of Project: Search for Neutrino Oscillations at LAMPF (E-645)
Prompt Neutrino Production at Fermilab (Fermilab E-613)

Persons in Charge: T. Y. Ling and T. A. Romanowski

Scientific and Professional Staff: T. Y. Ling, J. Fitch, J. Heimaster, J. Mitchell, T. A. Romanowski, C. J. Rush, E. Smith, and M. Timko.

Scope of Work

The primary activity of this group is the study of neutrino physics. The present effort is an experiment at LAMPF (E-645) to search for neutrino oscillations via the channels. $\nu_\mu \rightarrow \nu_e$ and $\nu_e \rightarrow \nu_e$. The experiment is designed to achieve sensitivities in Δm^2 ranging from 0.01 eV^2 to 20 eV^2 and $\sin^2 (2\theta)$ down to 0.001. The neutrino detector involves the use of scintillation or Cerenkov counters, proportional drift tubes, and other electronic techniques. This experiment is the main thrust of this activity and will continue for the next two years.

Their other neutrino experiment performed at Fermilab (E-613) was designed to study production of prompt neutrinos in proton nucleus interactions. In this experiment the incident proton beam interacted in targets with variable densities made of copper tungsten and beryllium. A magnetized and passive beam dump downstream of the target shielded the neutrino detector which consisted of a calorimeter made of lead plates and scintillator. A muon spectrometer composed of magnetized iron toroids and drift chambers followed the calorimeter.

Goals and/or Major Results to Date

The prototyping of the neutrino detector elements for the LAMPF experiment has been completed and mass production of these components is in progress. Their schedule calls for the start of the detector assembly at Los Alamos in the coming fall. A paper on a novel design of proportional drift tubes to be used for this experiment has been accepted for publication.

The data-taking phase of the beam dump experiment at Fermilab has been completed and the analysis of the data is nearly finished. The major results obtained in this experiment are the measurements of the ratios of the prompt neutrino fluxes of both ν_μ/ν_e and $\bar{\nu}_\mu/\nu_\mu$ which were found to be equal to nearly unity; the total and differential production cross section for $D\bar{D}$ and their A-dependence; and finally, the limits on the mass and rise times of the supersymmetric particles which could have been produced. Several of these results have been published in Physics Review Letters and others submitted for publication.

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OHIO STATE UNIVERSITY
Columbus, Ohio

Title of Project: Charm and Beauty Decays

Person in Charge: N.W. Reay

Scientific and Professional Staff: J. Dunlea, A. Gauthier, J. Heimaster, J. Kalen, S. Krivatch, S. Kuramata B. Lundberg, G. Oleynik, N. Reay, K. Reibel, C. Rush, R. Sidwell, and N. Stanton

Scope of Work

Experiment 531 used a hybrid emulsion spectrometer to investigate neutrino-induced production and subsequent decay and about 150 charm particles. Exposures were made in 1979 and 1981. First run results have been published; analysis of the second run will be complete within one year.

Experiment 653 is assembling a new hybrid emulsion spectrometer to investigate production and decay of 15,000 charm and 200 beauty particles generated in 800 GeV proton exposures at the Fermilab Tevatron.

Several types of ultrahigh spatial resolution detectors are being incorporated into a FASTBUS-based data acquisition system capable of low-rate emulsion and high-rate all-electronic modes of operation. A test run is scheduled for June 1984, and several data runs will occur between the end of 1984 and mid-1987.

Ohio State physicists conceived, and are leading both experiments, and have assumed responsibility for about half of the computer analysis and non-emulsion hardware. Their E-653 responsibilities include silicon chambers and the FASTBUS-based data acquisition system. They also are supervising the construction of the emulsion pouring and processing facility at Fermilab necessary to handle the 100 liters of emulsion approved for exposure.

Goals and/or Major Results to Date

E-531 measured D^0, $D\pm$, $F\pm$ and Λ_c^+ charm particle lifetimes, set the limit on $\nu_\mu \rightarrow \nu_\tau$ neutrino oscillations, measured cross sections for charm particle production by neutrinos, and has ruled out all suggested sources for neutrino-produced like-sign dimuons, except D^0 mass-mixing. The second run results will greatly improve statistics of published results.

E-653 plans to
1. improve charm and beauty lifetime measurements;
2. search for new ground and/or excited states of charm;

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OHIO STATE UNIVERSITY
Columbus, Ohio

3. examine rare decay modes such as $F \rightarrow \tau \rightarrow \ell + x$, which are needed in addition to beam dump results to establish the existence of the tau neutrino;
4. make a high statistics study of D^0 and B^0 mass-mixing and possible CP violation.

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1075

OHIO STATE UNIVERSITY
Columbus, Ohio

Award No. FG02-84ER40175

Title of Project: Electron-Positron Interactions

Persons in Charge: H. Kagan and R. Kass

Scientific and Professional Staff: T. Jensen, H. Kagan, R. Kass, P. Haas, J. Fitch, J. Heimaster, and C. Rush

Scope of Work

This group presently pursues two fields of research. The first consists of the study of electron-positron interactions at high energy. This study is performed using the CLEO detector at the Cornell Electron Storage Ring. In particular, they are interested in the study of the Υ family of resonances and the weak decay of B mesons. In addition, they are presently building a high precision vertex detector for the CLEO experiment.

The second activity pursued is a search for exotic forms of matter. This search, performed at the Nuclear Structure Research Laboratory of the University of Rochester, employs a new approach to such experiments. They use an all electrostatic charge selector in conjunction with a Van de Graaff accelerator to provide a mass-independent search for matter with fractional charges or anomalously large mass.

Goals and/or Major Results to Date

The CLEO collaboration has produced many new results in electron-positron interactions. Their main interests have been in the area of weak decays of B mesons. To date they have proved the existence of b-flavored hadrons, measured the semileptonic branching ratio $B^- \to e\nu X$, set limits on flavor changing neutral currents in the b-sector, set stringent limits on the fundamental coupling $(b^- \to u)/(b^- \to c)$ and set limits on the ratio of B^+/B^0 lifetimes.

Their goals in the near future include using the vertex detector to study charm and b decays. Also the exotic matter search should begin with studies of niobium, iron, lithium, and noble gases.

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UNIVERSITY OF OKLAHOMA
Norman, Oklahoma

Award No.: DE-AS05-80ER10629

Title of Project: High Energy Physics Group

Person in Charge: G. R. Kalbfleisch

Scientific and Professional Staff: G. R. Kalbfleisch, P. Skubic, S. E. Willis, J. M. Snow, and J. White

Scope of Work

They are pursuing basic research into the physics of charmed and bottomed elementary particles produced in hadron or photon interactions. The major objective of this task (to enable these studies) is the development of precision spaced measurements of particle tracks at the ten micron level. Integrated circuit masking technology allows the printing of fine lines (stripes) of diode junctions on a large silicon wafer (3 inch diameter). They are in contact with university and commercial vendors who are providing these devices. In addition, very sensitive (and inexpensive) amplifiers have been developed to electronically see the small signals (relative to the intrinsic noise) produced by charged particle tracks passing through the silicon wafers. The final products expected are thirty (or so) silicon devices (with some twenty thousand stripes) connected to some ten thousand amplifiers at a total cost of less than a million dollars, manufactured by commercial vendors.

Goals and/or Major Results to Date

Together with collaborators they have been approved to run experiment E-653 at Fermilab. Various R&D work has been completed. Analysis of the LBL silicon devices has been reported. Additionally, three CENTRONIC 8 cm^2 devices have been tested. Lecroy Research Systems has produced a hybridized preamp to the (OSU-OU) design. Final design of the beam SSD's has been completed; parts ordered; construction beginning. The precision time-of-flight (TOF) system is under way and crucial prototype testing of some hadron calorimeter avalanche tube modules has been done.

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1077

OKLAHOMA STATE UNIVERSITY
Stillwater, Oklahoma

Award No.: DE-AS05-76ER05074

Title of Project: Theoretical Studies in Weak, Electromagnetic, and Strong Interactions

Persons in Charge: K. A. Milton and M. A. Samuel

Scientific and Professional Staff: J. Reid, A. Sen, and G. Tupper

Scope of Work

This group carries out specific perturbative and nonperturbative field-theoretic calculations and developments so that experimental tests of theories of weak, electromagnetic, and strong interactions can be made and better theoretical understanding of these theories can be achieved. In the nonperturbative direction they are developing a new approach to lattice field theory called the finite element approximation, which will have important applications to the solution of lattice gauge theories, and they hope, to supersymmetry. Chromostatics represent a semiclassical approach to confinement which is being explored, and the hadronic implications of the Casimir effect are still under vigorous study. Perturbative work includes the following topics:

Production of Intermediate Vector Bosons, Locating Amplitude Zeros, Amplitude Zeros in Higher Order, Radiative Corrections to Pseudoscalar Meson Decays, Projection Operator Method, Decay of Z^0 into three gluons, Higgs Boson Production in Quark-Gluon Collisions, and Gauge Dependence of Green's Functions in the non-linear R_ξ Gauge.

Goals and/or Major Results to Date

One of the major results to date is the discovery of amplitude radiation zeros which can be used as a way of measuring the g value of the W boson and the quarks as well as measuring the quark charges in $p\bar{p} \to W^{\pm}\gamma X$. They have also studied radiation zeros in general and shown how to determine whether or not the zeros occur in the physical region. Nonperturbatively, they have shown that the Casimir effect provides a natural mechanism for quark and gluon condensates; that chromostatics implies bag formation in the color-singlet channel only for $q\bar{q}$, qqq, and gg systems; and that the finite element approach naturally solves the lattice fermion doubling problem.

In general, they hope in these and other directions to elucidate theory and facilitate contact with experiment.

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UNIVERSITY OF OREGON
Eugene, Oregon

Award No.: DE-AT06-76ER70004

Title of Project: Theory of Elementary Particles

Persons in Charge: P. L. Csonka, N. G. Deshpande, R. C. Hwa, M. J. Moravcsik, and D. E. Soper

Scientific and Professional Staff: I. Bigi, J. Chakrabarti, P. L. Csonka, N. G. Desphande, R. C. Hwa, M. J. Moravcsik, D. E. Soper, and X. R. Tata

Scope of Work

The research program of this group of investigators covers a broad variety of topics in high energy (elementary particles) theory and phenomenology. The fundamental aim of the research is to understand the nature of the forces that act among such elementary particles, an objective pursued by the international scientific community for some four decades by now but the attainment of which is yet to be achieved. Such an eventual understanding of these phenomena will broaden our scientific knowledge by a new dimension, will boost many other areas of science such as astrophysics, and will undoubtedly also result in revolutionary technolgical applications which cannot even be outlined in the absence of such an understanding.

Specifically, this group has made contributions to a number of different aspects of the field. Group theoretical models for unifying present fragmentary knowledge have been proposed and their implications outlined in terms of future experimental findings. Specific strong-interaction models have been proposed and related to existing experimental data. Some mathematical problems related to calculations with such models have been resolved. The scope of polarization experiments as tools for understanding particle dynamics has been elucidated and specific dynamical models have been tested. Novel methods of designing particle accelerators, using lasers and resulting in enormous savings in the cost of accelerator construction, have been proposed and their exploration on a pilot basis formulated.

Goals and/or Major Results to Date

The tangible output of the group is some 20-30 research papers per year published in the major refereed international journals. This is supplemented by contributions to international conferences and collaborations with theoretical and experimental groups in universities and laboratories around the world. Results of the research performed by the group are cited and utilized by many other research groups. Symmetry groups and phenomenological models widely used are associated with the names of some members of the group. Members of the group often visit other research groups for consultation and collaborative research.

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1079

UNIVERSITY OF PENNSYLVANIA
Philadelphia, Pennsylvania

Award No.: DE-AC02-76ER03071

Title of Project: Neutrino Studies and Nucleon Decay

Persons in Charge: E. W. Beier and A. K. Mann

Scientific and Professional Staff: K. Abe, K. Amako, E. Beier, D. Doughty, S. Durkin, L. Feldscher, S. Heagy, M. Hurley, A. Mann, M. Newcomer, R. Van Berg, H. Williams, and T. York

Scope of Work

The work of this group is focused on the fundamental properties and interactions of neutrinos and studies of the conservation of lepton number and baryon number. For the past several years, the principal effort of this group has been the construction and operation of a large, fine-grained neutrino interaction detector for the study of the elastic scattering of neutrinos and anti-neutrinos by electrons and by protons and various searches for neutrino oscillations. Additional effort has been made in the design of experiments to study nucleon decay and lepton number violating double beta decay. A new collaboration has recently been formed to upgrade the sensitivity of the Kamioka Nucleon Decay Experiment. This consists of implementing fast timing on the photomultiplier tubes of this 2.7 kton water Cerenkov detector and installing an active veto shield around the detector. When the upgrade is complete, the detector will have unequalled sensitivity to most hypothesized decay modes of nucleons.

Goals and/or Major Results to Date

The neutrino elastic scattering experiment has accumulated the world's largest sample of $\nu_\mu e$ and $\bar{\nu}_\mu e$ elastic scattering events (approximately 150 and 100, respectively). The experiment has been approved to double the data set in FY 1985. It will soon produce two new precision measurements of $\sin^2\theta_W$ with significantly better than ten percent accuracy from the electron and proton elastic scattering data. Work is proceeding on the upgrade of the Kamioka Nucleon Decay Experiment, with the goal of having the upgrade fully operational by the end of calendar year 1984.

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Title of Project: Selove group

Person in Charge: W. Selove

Scientific and Professional Staff: E. Gardella, W. Kononenko, W. Selove, B. Robinson, and G. Theodosiou

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Philadelphia, Pennsylvania

Scope of Work

This group does experimental high energy physics. The major recent and current efforts have involved (a) an experiment which recently completed data taking (E-609), the study of high transverse momentum jets, as a tool for studying parton-parton collisions at Fermilab, and (b) currently, design and development work for the D-zero proton-antiproton collider experiment at the Tevatron. The former experiment included major groups from ANL, Penn, Rice, and Wisconsin, with smaller collaborative efforts from Lehigh and Michigan. The D-zero experiment is a collaboration with currently 13 institutions and some 75 physicists. This experiment has a second-generation detector design, with some unique capabilities not present in the other collider detector at the Tevatron.

Goals and/or Major Results to Date

In E-609 the major goals were to find efficient methods for studying jets in hadron collisions and to measure di-jet cross sections as a significant test of QCD. These purposes have been accomplished; a recent report being submitted for publication gives the di-jet cross section for jet P_T values from 5 to 9 GeV/c at Fermilab energies.

In preparing the detector for this experiment, they devised the first 2-dimensionally segmented hadron calorimeter array and originated a calorimetry technique using scintillator and wave shifter bars, which then became the basis for all large hadron calorimeters built since then for study of hadron collisions.

In the D-zero experiment, their objectives have been to design, in collaboration with others, a powerful detector, or with some capabilities unique at Fermilab, which can study several different types of physics simultaneously. The D-zero detector design does have these capabilities, and has received very strong positive evaluations from many reviewers; they hope to be able to help bring this detector into operation at a very early date.

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Title of Project: Experimental High Energy Particle and Nuclear Physics

Person in Charge: S. Frankel

Scientific and Professional Staff: H. Brody, W. Frati, W. Molzon, E. Vella, and W. Zajc

Scope of Work

The group is engaged in two fields of experimental work: a) the study of ultrarelativistic particle physics in nuclei, and b) the study of QCD jets in p-p collisions. Both of these studies are carried out at the

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Philadelphia, Pennsylvania

CERN ISR (R807, the Axial Field Spectrometer Collaboration). It is the only American group to study nucleus-nucleus interactions at ultrarelativistic energies using the CERN ISR.

The ultrarelativistic nuclear physics research covers several activities: a) Studies of p-p, p-alpha and alpha-alpha interactions to learn about low pt particle production. These studies are concerned with the early time evolution of hadronic states, with models for soft QCD processes, and with studies of energy deposition as inputs to theories of deconfinement; b) Searches for deconfinement in alpha-alpha interactions; c) Studies of High pt phenomena in nuclei and the interplay of soft and hard processes in nuclei; d) Studies of phenomenological models for soft and high pt phenomena in nuclei. At present the group is completing analysis of alpha data from the 1980 ISR run and starting analysis of the data from the 1983 run. The latter run allows study of nuclei with uranium and sodium iodide calorimeters added in 1982 to the Axial Field Spectrometer (AFS).

The particle physics research mainly covers jet production at ISR energies measured with the uranium calorimeters and the AFS. The group is analyzing data accumulated in 1983 up to the closing of the ISR. It studies the complete even structure of hadron jets from $\sqrt{s}=31$ to $\sqrt{s}=63$ comparing results with QCD predictions, e^+e^- data, and models of jet production in hadronic matter.

Goals and/or Major Results to Date

The group was the first to measure alpha-alpha multiplicity distributions in the central region, correlate them with energy flow in the fragmentation region, and test various theories of soft particle production. It has made the only search for deconfinement, ie the search for a phase transition, by studies of strange non-strange particle ratios, and studies of K-2K and K-lamba Correlations in extremely high multiplicity nuclear collisions.

The group was the first to observe QCD jets at ISR energies, using calorimetry and unbiassed triggering.

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Title of Project: Colliding Detector Facility

Person in Charge: H. H. Williams

Scientific and Professional Staff: D. Bauer, D. Conner, J. Cooper, S. Hahn, N. Lockyer, M. Miller, R. VanBerg, and H. H. Williams

UNIVERSITY OF PENNSYLVANIA
Philadelphia, Pennsylvania

Scope of Work

The group is currently working on the Colliding Detector Facility at Fermilab. This detector, which combines excellent tracking capabilities with highly segmented calorimeter coverage over ±4 units of rapidity, is well suited to the study of proton-antiproton collisions at a center-of mass energy of 2 TeV. Searches for heavy new gauge bosons with masses up to 400-500 GeV and for heavy quarks with masses up to 100-125 GeV should be readily achievable. Current estimates of quark-quark and gluon-quark scattering cross sections indicate significant numbers of events will be observed with momentum transfers exceeding 200,000 GeV^2. Searches for supersymmetric particles and precise measurements of the $W^\pm$ and Z^0 masses and widths will also be of great interest.

To date, the University of Pennsylvania contribution to CDF has focussed on the calibration and monitoring for the scintillation calorimetry. This includes responsibility for the photomultiplier bases and high voltage power supplies, Xenon flasher systems, source measurements for monitoring the long term stability of the calorimeters, and the initial test beam calibration. On-line software is being provided for the above systems and for monitoring and calibration using $\bar{p}p$ interactions. The group is also providing specifications and testing for the photomultiplier electronics, particularly regarding the electronics calibration.

Goals and/or Major Results to Date

Production and testing of the scintillator calorimeters and the above calibration systems is progressing satisfactorily. It is anticipated that all of the scintillation calorimetry will be tested and installed by mid-1985.

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Title of Project: Quarkonium Production in Hadron Interactions at Fermilab

Person in Charge: J. W. Cooper

Scientific and Professional Staff: D. A. Bauer

Scope of Work

This group's primary activity is the study of charmonium production in hadronic interactions at Fermilab. They used the Chicago Cyclotron Particle Spectrometer to observe ω, ϕ, $\Psi(3100)$, and $\Psi'(3685)$ production by means of their dimuon decays. They could also observe directly the hadronic production of the charmonium χ states, since these states decay via $\chi \rightarrow \Psi + \gamma$ and their apparatus contained a large lead glass array to detect photons. Charmonium χ production was their main focus since different χ states should be produced in quark-antiquark versus gluon-gluon mechanisms. They used π^- and proton beams in their investigation of the relative strengths of these two production mechanisms.

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Philadelphia, Pennsylvania

Goals and/or Major Results to Date

They have observed substantial hadronic χ production, finding that one-third of all $\psi(3100)$ are produced via χ states in both π^- Be collisions and p Be collisions. The principal result is that the $\chi(3555)$ state is predominantly produced in p Be interactions, while both $\chi(3510)$ and $\chi(3555)$ are seen in π^- Be interactions. This observation is consistent with the interpretation that simple gluon-gluon fusion into color singlet states is the dominant production mechanism in proton interactions.

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Title of Project: Neutrino Physics and Cosmology

Person in Charge: S. A. Bludman

Scientific and Professional Staff: S. A. Bludman, Y. Hoffman, H. Lee, E. Myra, G. Steigman, and T. Gaisser

Scope of Work

Applications of Elementary Particle Theory to Cosmic Phenomena:

1. Role of Neutrinos in Stellar collapse and Supernova Explosions: Obtaining a supernova explosion from the collapse of massive stars requires careful calculation of neutrino production and trapping, of the nuclear equation of state, and of the coupling between neutrino radiation transport and shock hydrodynamics;

2. Flux and Angular Distribution of Neutrinos made in the Atmosphere by Cosmic Rays: These neutrinos are the principal background in nucleon decay experiments, a source for neutrino experiments over terrestrial flight paths, a cosmic-ray benchmark, and a pedestal from which to search for extraterrestrial neutrinos from astrophysical sources;

3. Dynamic Evolution of the Large Scale Structure of the Universe: Deep sky surveys plus numerical simulations plus particle theory test GUTs and inflationary cosmology.

Goals and/or Major Results to Date

1. Thermal stiffening and shock ejection is probably the mechanism for mass blow-off. The evolved iron core of the massive star needs to be relatively cool and small;

2. The flux and angular distribution of atmospheric neutrinos serves to calibrate and intercalibrate underground detectors and to set limits on neutrino oscillations;

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Philadelphia, Pennsylvania

3. If large scale structure evolved by gravitational instability, the universe cannot be dominated by unclustered dark matter and needs to be open, rather than flat.

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Title of Project: High Energy Theory

Person in Charge: G. Segre

Scientific and Professional Staff: G. Segre, S. Bludman, P. Langacker, P. Steinhardt, Y. Hosotani, B. Sathiapalan, Y. Ahn, N. Cao, L. Jensen, P. Lindblom, J. Socolar, and S. Umasankar

Scope of Work

The aim is to study various aspects of the theory of elementary particles. Primary efforts have been in both the theory and phenomenology of electroweak models and of grand unified models. They have been interested in explaining and correlating the results of performed experiments and in the planning of new ones.

Among the areas worked on are neutrino physics, calculation of masses and mixing angles, CP violation, models of supersymmetry, and proton stability.

A recent strong interest of the group has been the physics of the early universe as a testing ground for theories of elementary particles. Some of the problems studied in this area are expansion of the universe, inflationary models, high temperature field theory, generation of the baryon asymmetry of the universe, and constraints on supersymmetric models.

Goals and/or Major Results to Date

They plan to continue to work in the frontier areas of high energy physics along many of the same lines followed in the past years. In particular, they wish to maintain or extend their impact on work in electroweak models, GUT's, and problems of the early universe, the areas in which their most significant work has been done in the past few years. This may lead them more into the areas of supersymmetry and supergravity as well.

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UNIVERSITY OF PENNSYLVANIA
Philadelphia, Pennsylvania

Award No.: DE-AC02-81ER40012

Title of Project: Study of High Energy Physics Underground

Person in Charge: K. Lande

Scientific and Professional Staff: M. Cherry, C. K. Lee, R. Steinberg, S. Corbato, and D. Keida

Scope of Work

The purpose of this project is to carry out a very sensitive search for magnetic monopoles using a very large liquid scintillator hodoscope in a deep underground location. The detector is a 140 ton liquid scintillator hodoscope in the form of a hollow box, 8m high, 8m wide, and 16m long. The hodoscope consists of 200 individual modules, each 30cm by 30cm by 8m. The detector is located 4850 ft. below the surface of the earth in the Homestake Gold Mine in Lead, South Dakota. In addition to the monopole search, the detector is also being used to study the transmission of high energy neutrinos through the earth, look for neutrinos from collapsing stars and measure the composition of very high energy cosmic rays by studying the multiplicity and transverse momentum distribution of high energy muon secondaries resulting from the interaction of cosmic ray primaries with the upper atmosphere.

Goals and/or Major Ressults to Date

Half of the scintillation hodoscope has recently been turned on and preliminary data has been acquired on the cosmic ray muon fluxes and angular distributions. A careful calibration of each detector module has also been carried out. Based on this calibration, it appears that the detector will have an effective threshold below 1/10 minimum ionization (5 MeV) and is able to discriminate against local background at this threshold. These results not only instill confidence in the ability of this device to search for slow, lightly ionizing monopoles, but suggest that this type of detector configuration may also be able to investigate sources of low energy neutrinos such as the sun.

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UNIVERSITY OF PITTSBURGH
Pittsburgh, Pennsylvania

Award No.: DE-AC02-80ER10667

Title of Project: Study of Large P_T Direct Photon Production at the ISR

Persons in Charge: W. E. Cleland and J. A. Thompson

Scientific and Professional Staff: Y. Choi, W. E. Cleland, R. Kroeger, M. Sullivan, and J. A. Thompson

Scope of Work

This work is carried out with the Axial Field Spectrometer (AFS) collaboration at CERN. This collaboration is studying high P_T phenomena in general, including single particle and jet production processes, high E_T events, direct photon production at high P_T, and properties of jets. In addition, states produced with very small momentum transfer (double pomeron production) are studied, as well as possible anomalous electron or photon production at low P_T. This group is particularly interested in direct photon production.

The Pittsburgh group is involved in three main studies:

1. Photon and π^0 production at ~11^0 and $P_T > 2\text{-}3$ GeV/c, and correlations of charged secondaries with respect to trigger π^0's. Detectors: small hexagonal uranium-scintillator electromagnetic calorimeter at 11^0 to beam; AFS axial drift chamber, with acceptance $|y| < 1.2$.

2. Comparison of photon production at 90^0, $P_T > 2$ GeV/c, in pp and $\bar{p}p$ collisions. Detectors: two NaI arrays mounted on inside face of AFS uranium calorimeters. The NaI/uranium detector combination allows studies of 20 MeV-5 GeV photons.

3. Comparison of observed photon production at 90^0, $P < 200$ MeV/c, with that expected from known sources. Detectors: NaI detectors, described above; AFS central drift chamber (for removal of apparent photons associated with charged tracks).

Goals and/or Major Results to Date

1. Analysis of the data from the small-angle hexagon calorimeter shows that the QCD bremsstrahlung contribution to direct photon production is smaller than expected. A study of correlations of π^0's with charged tracks gives evidence for the vector nature of the gluon and constrains phenomenological descriptions of small-angle, high P processes.

2. Preliminary results from a fraction of the $P_T > 2$ GeV/c, 90^0 direct photon production show no striking differences between pp and $\bar{p}p$ collisions; completion of this project requires further data analysis and systematic bias studies.

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Pittsburgh, Pennsylvania

3. Studies of the low energy photon spectrum are in progress; results are not yet available.

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Title of Project: Direct Photon Production at the Tevatron (E-706)

Persons in Charge: E. Engels, Jr. and P. F. Shepard

Scientific and Professional Staff: W. E. Cleland, D. Coon, E. Engels, P. Shepard, J. Thompson, D. Plants, S. Mani, Y. Yang, and R. Wilkins

Scope of Work

The principal activity of this task is a study of direct photon production along with accompanying hadron production at the Tevatron. Their group is assembling a silicon strip detector system of 6000 channels to instrument the production target and to provide tracking information for a large magnetic spectrometer, a part of the apparatus for the experiment. The experiment, which is a collaboration involving Fermilab, the University of Pittsburgh, Michigan State, Penn State, the University of Rochester, and the University of Minnesota, is expected to begin data taking in February 1986. As a part of this activity, they are developing the technology to produce room temperature silicon strip detectors with the Westinghouse R and D Center in Pittsburgh. At present, these detectors are only available through foreign vendors. As part of a longer term effort, they are also investigating the possibility of building a new type of silicon particle detector known as a crogenic charge storage detector which operates at liquid He temperatures. This device stores the charged carriers produced by fast charged particles in shallow impurity traps. Because of this local charge storage it offers the possibility of producing detectors with far fewer external connections and electronic amplifier channels.

Goals and/or Major Results to Date

This task began with the approval of E-706 at FNAL. Goals include the continued investigation of direct photon physics if that is indicated by the initial effort at FNAL. They are also interested in the use of the spectrometer for the investigation of the production of charm and beauty. In connection with the detector development, they have successfully demonstrated the use of single element cryogenic devices as particle detectors.

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UNIVERSITY OF PITTSBURGH
Pittsburgh, Pennsylvania

Title of Project: Search for Fractional Charge in Semiconductors

Person in Charge: D. Coon

Scientific and Professional Staff: D. Coon and S. Gunapala

Scope of Work

The work involves the development and evaluation of a new means of searching for fractional charge impurities in semiconductors. The method is based on the prediction of the electronic energy levels of fractional charge impurities in semiconductors. The experimental approach employs a combination of field ionization techniques and far infrared spectroscopy. The approach is electronic and spectroscopic so that mechanical sample size constraints and mechanical techniques common to many other searches are avoided. The samples are integral components of electronics. This feature results in excellent opportunities for signal averaging which they will exploit.

Goals and/or Major Results to Date

They have developed a liquid helium cooled monochromator system and employed this system in tests of their approach. The tests have involved integer charge impurities which do not require as much cooling as do fractional charge impurities. The work to date has been successful in implementing new techniques which combine field ionization and infrared spectroscopy.

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PRINCETON UNIVERSITY
Princeton, New Jersey

Award No.: DE-AC02-76ER03072

Title of Project: Muon Scattering

Person in Charge: F. C. Shoemaker

Scientific and Professional Staff: F. C. Shoemaker and M. Arneodo

Scope of Work

This program started with Fermilab experiment E-203 which was mounted in the fall of 1977 and ran in the spring of 1978. The multi-muon spectrometer is a distributed iron target-calorimeter-magnetic spectrometer with a high target luminosity (5 kg/cm^2) and the ability to take muon beam intensities of a few times 10^6 muons per second. A notable feature is that the track chambers are sensitive in the beam region, allowing complete reconstruction of multi-muon events.

The present program is to move the multi-muon spectrometer to the new muon laboratory which will have muons of higher energy, from the Tevatron. The multi-muon spectrometer will be improved by the addition of drift chambers to give the Y coordinate in the central region (beam and vertex) and additional trigger counters.

Goals and/or Major Results to Date

E-203 produced the first measurements of J/ψ muoproduction and polarization, the first measurements of charm muoproduction and its contribution to scale non-invariance; also, a limit on Υ muoproduction and a lower limit on the mass of a neutral heavy lepton; further, a high statistics measurement of the nucleon structure function in iron and a study of rare processes induced by muons. The goals of E-640 are to study, with muons with energy up to 600 GeV:

1. Inelastic muon scattering and the determination of the nucleon structure function up to $Q^2 = 600\ (GeV/c)^2$
2. Production of high mass vector mesons
3. Production of heavy quark states
4. Heavy lepton production
5. Study of final states with four or more muons.

Experiment E-203 demonstrated the ability of the multi-muon spectrometer to effectively explore all aspects of this list of goals. The proposal for this experiment requested approval of a study of weak-electromagnetic interference, which would produce an asymmetry of 3-4 percent at $Q^2 = 400\ (GeV/c)^2$, and the muon beam is being constructed so that the helicity of the muons may be controlled. However, approval of this phase of the experiment was deferred.

Preliminary tests of the apparatus will take place in the spring of 1985.

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Title of Project: A Study of CP Violation in the Neutral Kaon System

Person in Charge: G. D. Gollin

Scientific and Technical Staff: G. D. Gollin, A. Fruchter, and G. Grazer

Scope of Work

This group is studying CP violation in $K_L \to 2\pi^0$ and $K_L \to \pi^+\pi^-$ decays. A precise determination of η_{00}/η^{+-} tests the predictions of the standard model, and less orthodox models, of the weak interactions. η_{00}/η^{+-} is expected to be different from unity by perhaps a percent. The present effort involves two experiments, both utilizing a drift chamber spectrometer and an 804-block lead glass array in the twin neutral beam in the meson area at Fermilab. The first experiment, E-617, finished taking data in June 1982. The second, E-731, will run in 1985 E-617 is a collaboration between the University of Chicago, Princeton, and CEN Saclay; E-731 involves groups from Chicago, Fermilab, Princeton, and Saclay.

Goals and/or Major Results to Date

E-617 recorded approximately 3000 $K_L \to 2\pi^0$ decays. The data analysis will be complete by summer 1984. They will report measurements of η_{00}/η^{+-}, the magnitude of η^{+-}, the radiative decay width of the $K^*(892)$, and the branching ratio for $K_L \to \gamma\gamma$. The 5 percent background under the $K_L \to 2\pi^0$ signal is from $K \to 3\pi^0$ decay where two photons were lost. Their preliminary result on η_{00}/η^{+-} is that $\eta_{00}/\eta^{+-} = .989 \pm .015$ where the quoted error is statistical. Systematic errors are comparable to statistical errors and are under investigation.

E-731 will run at the Tevatron in 1985. The new beamline and higher-acceptance detector will increase their $K_L \to 2\pi^0$ event rate by a factor of 30. A set of photon anticounters to be built at Princeton will substantially reduce backgrounds. They expect to record 100,000 $K_L \to 2\pi^0$ decays and determine η_{00}/η^{+-} to an accuracy limited by statistics. Testing of prototypes for a beam Cerenkov counter and for photon anticounters is in progress. Construction will take place during the spring and summer of 1984.

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PRINCETON UNIVERSITY
Princeton, New Jersey

Title of Project: e^+-e^- Interactions

Person in Charge: P. A. Piroué

Scientific and Professional Staff: J. A. Bakken, D. Stickland, R. L. Sumner, A. J. S. Smith, M. Isaila, and C. Bopp

Scope of Work

This group is part of the LEP3 collaboration which is building a $60M detector for the new 100 GeV e^+e^- collider (LEP) now under construction at CERN, Geneva, Switzerland, and scheduled to be completed in 1988.

The responsibility of the Princeton group is the construction of a $12M electromagnetic calorimeter which uses as absorber 12,000 crystals of BGO (bismuth germanate). This responsibility is shared with LAPP (Laboratoire d'Annecy de Physique des Particules) which has, as primary task, the construction of the mechanical parts whereas Princeton is primarily responsible for the electrical part, i.e., the complete readout system of the 12,000 crystals.

Goals and/or Major Results to Date

The LEP3 detector is optimized for the following goals:

1. Perform precise measurements in the framework of the Standard Model (e.g., Z^0 physics) and to search for scalar particles, such as Higgs, by missing mass techniques of the type $e^+e^- \rightarrow \ell\ell + X$.
2. Explore new phenomena (not predicted by theory) by precise measurements of e, μ, γ, and hadron jets.

The BGO calorimeter which consists of 12,000 BGO crystals (~2.5 x 2.5 x 24cm) placed in a 0.5T magnetic field is expected to produce signals ranging from ~100 MeV to 100 GeV which will be read with a precision better than 1 percent over the whole range. A readout system has been designed, based on the large scale use of single chip microcomputers, which exploits the local intelligence available at each crystal in order to reduce the amount of cabling needed.

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Title of Project: Hadronic Interactions

Person in Charge: P. A. Piroué

Scientific and Technical Staff: D. P. Stickland, R. L. Sumner, C. A. Bopp, M. V. Isaila, and H. Edwards

PRINCETON UNIVERSITY
Princeton, New Jersey

Scope of Work

This group has been studying hadronic interactions since its inception in 1978. Early work concerned the production of hadrons, and later muons, at high P_T in proton-nucleus collisions with protons of up to 400 GeV energy. An unexpected observation was that the hadron production cross sections were found to have an atomic mass (A) dependence which grew with P_T, eventually leveling off to proportional to $A^{1.1}$. The first observation of direct muon production was made in the Chicago-Princeton experiment, E-100, at Fermilab. A natural extension of this work was the study of dimuon production and in E-325 the scaling of continuum muon pair production with M^2/s was established. In 1979, a further Fermilab experiment, E-258, extended the high P_T particle production studies to pion-nucleus collisions.

In 1980, they commenced E-326, a high statistics study of dimuon production in pion-nucleus interactions, once again in collaboration with the University of Chicago. This experiment was run in 1980-82 and they are now completing its analysis.

Goals and/or Major Results to Date

Experiment E-326 is a tool for studying the continuum muon-pair production mechanism. They have good acceptance for high mass pairs and for pairs produced with high P_T. Production of muon pairs at high P_T was not expected in the Drell-Yan model and is currently explained by the presence of initial state interactions in the colliding hadrons. This experiment is thus complementary to the work of the E-615 Chicago-Princeton group studying the same mechanism but at large X_F.

Early results from E-326 which have been published confirmed the target Atomic Number (A) dependence of continuum production as being proportional to A^α where $\alpha = 1$, and the non-rise of $\langle P_T^2 \rangle$ with $A^{1/3}$. This second result is significant since some models of the initial state interactions would require a measurable rise in $\langle P_T^2 \rangle$ with $A^{1/3}$ in this experiment.

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Title of Project: Fermilab Experiment 615, A Study of Muon Pairs Produced in $\pi^\pm$Nucleus Interactions

Person in Charge: K. T. McDonald

Scientific and Professional Staff: C. Biino, J. F. Greenhalgh, W. C. Louis, K. T. McDonald, S. Palestini, F. C. Shoemaker, and A. J. S. Smith

PRINCETON UNIVERSITY
Princeton, New Jersey

Scope of Work

They are investigating the production of $\mu^+\mu^-$ pairs in $\pi^\pm$-nucleus in reactions via the Drell-Yan mechanism. This electromagnetic interaction results from quark-antiquark annihilation and is well understood. This allows a determination of the motion of the quarks and antiquarks within the pion and the nucleus. E-615 puts particular emphasis on muon pair production in the forward direction, which must result from a configuration, in which a single antiquark inside the pion carries ~ 90 percent of the pion momentum. In this kinematic limit, one expects significant QCD corrections to the simple quark model, some of which were observed in previous experiment E-444. They are pursuing the question of QCD corrections in the form of scaling violations by a comparison of production rates at 75 GeV and 250 GeV beam energies. Also, they will accurately measure the departure of the μ pair decay angular distribution from $1 + \cos^2\theta$, which was the original indication of the QCD corrections.

Goals and/or Major Results to Date

Princeton University built three major hardware systems for E-615: 7 bands of scintillator hodoscopes; 16 planes of drift chambers; and the trigger processor. The experiment had a brief test run in 1982. Results of this run are nearly ready for publication and confirm the departure of the decay angular distribution from $1 + \cos^2\theta$. The main data run is now under way. The 75 GeV run is complete and analysis already well advanced. In 1984 they should have a major exposure with 250 GeV $\pi^\pm$ beams.

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Title of Project: Brookhaven Experiment 732 - A Search for New Particles in the Reaction $\pi^- p \to n + \gamma$'s at 13 GeV/c

Person in Charge: K. T. McDonald

Scientific and Professional Staff: A. M. Halling, C. G. Lu, K. T. McDonald, A.J.S. Smith, and M. Ye

Scope of Work

They have searched for the new particles decaying to $\gamma\gamma$, 3γ, 4γ which are produced in $\pi^- p \to n + \gamma$'s near threshold. With a 13 GeV/c beam they are sensitive to the mass range 2.0 - 3.5 GeV/c^2, which encompasses possible production of the η_c meson. In 1978 there was a report of production of a 2γ resonance of mass 2.85 GeV in $\pi^- p$ at 40 GeV/c, which at that time was considered as a candidate for the η_c.

PRINCETON UNIVERSITY
Princeton, New Jersey

They built a multi-photon detector which emphasizes good photon position resolution, moderate energy resolution, and vetoing of soft photons from π^0 decay over 4π solid angle.

Goals and/or Major Results to Date

They find no evidence for production of narrow resonances with mass above 2 GeV/c decaying to $\gamma\gamma$. A limit of $\sigma B \sim 80$ pb is set at mass 2.95 GeV/c. These results have been accepted for publication in Physics Letters. Further results, setting a limit on J/ψ production and decay to e^+e^- should be available shortly.

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Title of Project: Studies for a Possible Future Experiment

Person in Charge: V. L. Fitch

Scientific and Professional Staff: V. L. Fitch and A. Fruchter

Scope of Work

They are carrying out some very preliminary assessments of the feasibility of detecting the metric field component of gravity, i.e., the component of the acceleration due to the spinning earth,

$$\frac{\vec{v} \times (\vec{v} \times \vec{\zeta})}{c} \quad \text{where } \vec{\zeta} = \frac{2G(r \times J_{\bullet}}{cr^2}$$

Goals and/or Major Results to Date

They have just started to assemble some apparatus for the purpose of measuring relevant noise levels.

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Title of Project: $K^+ \rightarrow \pi^+$ + Missing Neutrals (E787 at Brookhaven)

Person in Charge: A. J. S. Smith

Scientific and Professional Staff: A. J. S. Smith, W. C. Louis, D. R. Marlow, P. D. Meyers, and M. Selen

Scope of Work

Along with physicists from Brookhaven, Carnegie-Mellon, Columbia, Princeton, and TRIUMF, they have designed an experiment to measure the rare decays

$K^+ \to \pi^+ + X^0$ where X^0 is a system of electrically neutral, weakly interacting particles. The experiment is designed to reach a level of sensitivity better than 2.10^{-10} in branching ratios for the mode $K^+ \to \pi^+\nu\nu$, and 4.10^{-11} for the two-body decay $K^+ \to \pi^+ X^0$, where X^0 is a light invisible particle. Both of these limits are three orders of magnitude beyond those of present experiments.

The reaction $K^+ \to \pi^+ + X^0$ is one of the few in which phenomena involving a mass scale well above 100 GeV can be explored at existing accelerators. In the context of the standard model, the decay $K^+ \to \pi^+\nu\bar{\nu}$ proceeds via a second order weak interaction, theoretical estimates of the branching ratio ranging from 10^{-9} to 10^{-10}. Additional light neutrino flavors enhance the branching ratio, but unless there are a large number of them, a definitive conclusion is unlikely. More exciting, many supersymmetric theories include light particles (nuinos, photinos), and it is possible that the decay $K^+ \to \pi^+ \tilde{\gamma}\tilde{\gamma}$ could be lurking just below the present limit of $2 \cdot 10^{-7}$. Another intriguing possibility is the observation of a generation-changing two-body reaction $K^+ \to \pi^+ X^0$, where now X^0 is a single neutral.

The above conjectures are speculative, except for the small value form second-order weak processes if only three generations are present. Therefore, observation of anything above a few times 10^{-10} in branching ratio indicates that something new is present, eventhough it might not be possible to identify which particular interaction is responsible. Non-observation at the level of 2.0^{-10}, though not as earthshaking, nevertheless would set severe constraints on many proposed models.

Goals and/or Major Results to Date

The experiment was approved in November 1983 and given very high priority by the Brookhaven Program Committee and the Laboratory Directors. At present, the detector is being designed in detail and the testing of prototypes is under way. The heart of the experiment is a range-energy telescope, which also serves to identify pions by seeing the $\pi^+ \to \mu^+ \to e^+$ decay sequence. Princeton will very likely be responsible for the design and construction of this experiment and data analysis.

The experiment should be ready for the first data by summer 1986.

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Title of Project: Theory

Person in Charge: C. G. Callan

Scientific and Professional Staff: F. Brown, C. Callan, P. Woit, and L. G. Yaffe

PRINCETON UNIVERSITY
Princeton, New Jersey

Scope of Work

The task of the theory subgroup is to pursue quantum field theory problems raised by developments in elementary particle physics. They are currently working on some novel lattice approximation methods for quantum chromodynamics and exploring some recently discovered properties of grand unification magnetic monopoles which promise to have important phenomenological and cosmological implications.

Goals and/or Major Results to Date

The lattice approximation studies have yielded results which include: the construction of a workable lattice topological charge which was then used in Monte Carlo explorations of the theta-dependence of vacuum quantities; the development of a new framework for computer determination of the large-N (where N is the number of colors in the QCD gauge group) limit of the wave functions of the QCD vacuum and low-lying hadron states. One of the motivations for pursuing these difficult problems is the realization that the vacuum angle (theta) and the number of color degrees of freedom are virtually the only physically variable parameters in the QCD Lagrangian. By exploring how the physics of QCD responds to variations of these parameters, they hope to gain insights which will make it possible to develop calculational methods applicable to the "real-world" version of the theory.

The magnetic monopole studies have yielded results which include the discovery of the remarkable phenomenon of monopole catalysis of proton decay as well as the development of a method, based on the Skyrme soliton model of hadrons, for computing detailed cross-sections and branching ratios for this phenomenon. Proton decay catalysis is of importance for the design and interpretation of monopole search experiments and, via neutron stars, provides a completely new category of sensitive cosmological limits on monopole abundance. To satisfy the needs of these applications, reasonably firm catalysis cross-section estimates are needed. The monopole problem provides a new and challenging arena in which to do strong interaction physics and their current efforts are devoted to an attempt to develop methods good enough to provide at least semi-quantitative estimates of important cross sections.

Active research on these topics will continue into at least the near-term future.

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PRINCETON UNIVERSITY
Princeton, New Jersey

Award No.: DE-FG02-84ER40174

Title of Project: The Construction of a Cylindrical Drift Chamber for Experiment 787 at BNL

Person in Charge: W. C. Louis

Scientific and Professonal Staff: W. C. Louis

Scope of Work

The objective of this project is the construction of a detector to study rare kaon decays at Brookhaven National Laboratory. Kaon Decays have been vital in revealing new physics and in enriching our understanding of the weak and electromagnetic interactions, and they allow the measurement of higher order weak effects and possible new phenomena. The detector will have the ability to measure the momentum, energy, and range of the kaon decay products and to suppress backgrounds to the level of one in ten billion. Overall, the detector should greatly enhance our knowledge of rare kaon decays.

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PURDUE UNIVERSITY
West Lafayette, Indiana

Award No.: DE-AC02-76ER01428

Title of Project: Experimental High Energy Physics

Person in Charge: J. A. Gaidos

Scientific and Professional Staff: I. L. Beltrami, J. A. Gaidos, D. S. Koltick, F. J. Loeffler, U. Mallik, R. L. McIlwain, D. H. Miller, T. R. Palfrey, L. K. Rangan, G. H. Sembroski, E. I. Shibata, R. B. Willmann, and C. L. Wilson

Scope of Work

This group is engaged in high energy physics research utilizing accelerator and nonaccelerator techniques. Currently the major experiments taking data include the High Resolution Spectrometer in the PEP-12 program at SLAC and the Harvard-Purdue-Wisconsin proton-decay detector in a Utah mine. Development and construction for projects to study TeV astrophysical gamma rays and TeV neutrinos (DUMAND) are well under way.

Goals and/or Major Results to Date

Products of high energy e^+e^- annihilations are being precisely measured by the HRS detector at SLAC, making possible a more detailed analysis of D^*, D, F charmed resonances than heretofore attained. Continued running and analysis will contribute a more thorough understanding of the new spectroscopy. The HPW proton-decay detector is particularly sensitive to muonic final states and will continue to search for various nuclear decay channels involving two or more muons. Present limits for the non-conservation of baryon number are beyond those suggested by simple grand unification schemes. Very high energy processes, available only in astronomical sources, will be studied by detecting the TeV neutrinos and photons from hadronic and electromagnetic interactions.

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Title of Project: Fundamental Particle Theory

Person in Charge: R. H. Capps

Scientific and Professional Staff: L. A. P. Balazs, R. H. Capps, T. E. Clark, E. Fischbach, N. Fuchs, T. K. Kuo, J. Hiller, T. Kephart, and N. Nakagawa

PURDUE UNIVERSITY
West Lafayette, Indiana

Scope of Work

This group pursues theoretical research in various areas of fundamental particle physics. In addition, various of the staff members supervise graduate students. The number of students in the program now is eight, and usually is close to this number. The work of the group members is sufficiently varied to give students a wide choice of research areas. There are many interactions among the staff members, research associates, and graduate students in informal and formal discussions, and in the weekly theoretical seminar and weekly journal club started recently. Frequently, research collaborations result from these interactions.

The group frequently invites outside theorists for short visits. About half of the theoretical seminars are given by outside speakers. There is an ongoing interaction of the group with the experimentalists in particle physics here, both in informal discussions and by mutual attendance at the particle theory seminar, the particle experimental seminar, and journal club.

Goals and/or Major Results to Date

During the last year, members of the group have made important contributions to a variety of research fields, including grand unified theories, possible cosmological effects on particle interactions, quark masses in chiral theories, and quark loop effects on hadron Regge trajectories. The results on grand unified theories involve several topics, including chiral anomalies, supersymmetry, horizontal gauge groups, and modifications that lead to a longer proton lifetime. Much of the work done involves problems at the forefront of present-day particle physics.

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Title of Project: An Experimental High Energy Physics Program

Persons in Charge: V. E. Barnes, D. D. Carmony, A. F. Garfinkel, and L. J. Gutay

Scientific and Professional Staff: A. Bujak, R. S. Christian, R. J. De Bonte, A. Di Virgilio, A. T. Laasanen, and B. C. Stringfellow

Scope of Work

This task supports experimental research on the interactions of elementary particles at high energies. The principal aim of these studies is to discover the complete set of fundamental particles and to understand in detail the basic forces of nature. Of particular current interest are (a) a study of bound states of charm quarks; and (b) an investigation of the state of hadronic matter at abnormally high energy density.

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PURDUE UNIVERSITY
West Lafayette, Indiana

Goals and/or Major Results to Date

In low energy neutrino interactions, they made the first observation of neutral currents in exclusive reactions, measured the isovector form factor M_A, and made a detailed isospin analysis of single pion production; while at high energy, they made the first measurement of the structure functions of protons using antineutrinos and determined the coupling of the strange to charmed quarks.

They have pioneered the study of π-π interactions, tested vector dominance and current algebra, as well as discovered the pion exchange dominance of Gamow Teller transitions. They established the existence of compressed hadronic matter and measured its size and limiting temperature as well as finding evidence for a hadronic phase transition at the critical point.

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Title of Project: Hadrons as the Relativistic Bound States of Baryons and Antibaryons

Person in Charge: M. Sugawara

Scientific and Professional Staff: V. M. Ayres

Scope of Work

The purpose of this project is to show that all the observed hadrons can be understood as the relativistic bound states of the non-strange, strange, charmed, bottom, and top baryons. For this purpose, they first eliminate the gluons at least partially by means of canonical transformations to generate the direct fermion-field interactions, where the leading interaction becomes the invariant four-fermion interaction. They then study the Bethe-Salpeter (BS) equation in which the irreducible kernel is due to the above invariant four-fermion interaction.

Goals and/or Major Results to Date:

The above canonical transformations determine not only the bound-state Hamiltonian which is responsible for all the hadrons, but also the decay Hamiltonian which explains all the strong decays of these hadrons. It is found that this decay Hamiltonian explains the OZI rule.

When they assume that the BS kernel is independent of the masses of the baryons bound in these bound states, they can determine this BS kernel based upon the known masses of the ordinary, strange, and charmed mesons, which then allows them to evaluate the bottom and top meson masses. They find that the toponium state becomes unstable against the decay into a pair of vector top mesons which are the narrow states that can decay into πK.

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1101

RICE UNIVERSITY
Houston, Texas

Award No.: DE-AS05-76ER05096

Title of Project: High Energy

Person in Charge: G. C. Phillips and J. B. Roberts, Jr.

Scientific and Professional Staff: S. D. Baker, G. S. Mutchler, H. E. Miettinen, M. D. Corcoran, J. A. Buchanan, and J. M. Clement

Scope of Work

The research is directed towards studies of the hadronic, strong interactions at high energies. It is especially interested in the investigation of phenomena such as jet formation, high multiplicity particle production, and the role of spin in high energy hadron-hadron and hadron-nucleus collisions by using both polarized proton beams and targets. Studies of proton spin-polarization effects were carried out earlier at ANL/ZGS at 1-12 GeV energies and are to be extended to AGS energies soon. A polarimeter for the polarized proton beam has been constructed and installed at AGS. At FNAL, an approved collaborative experiment will study proton spin polarization effects at the Tevatron using a beam formed by Λ decay. Experiments at FNAL have studied jet formation, and interesting multiparticle production effects have been observed for p-nucleus collisions.

Goals and/or Major Results to Date

Progress has been made in the jet studies of FNAL E-609 and includes interesting results for p-nucleus interactions. The spin studies have progressed during the year by: (1) completion of proton spin polarimeter construction, its calibration at Indiana University's Cyclotron Facility, and its installation at AGS/BNL; (2) approval of E-704, the first generation collaborative polarized proton experiment at FNAL.

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ROCKEFELLER UNIVERSITY
New York, New York

Award No.: DE-AC02-81ER40033

Title of Project: CERN Program

Person in Charge: R. Cool

Scientific and Professional Staff: R. Breedon, T. Cox, J. Linnemann, R. Rusack, G. Snow, and C. von Gagern

Scope of Work

The group at CERN has been involved in two experimental efforts: one at the Intersecting Storage Rings (ISR) and the other at the SPS Collider. The ISR experiment has had successful data runs with p-p and $\bar{p}$-p collisions and recently with α-α, p-α, and d-d. A wide variety of high energy topics have been under investigation, including production of high mass electron pairs (Upsilon meson mass and above), inclusive π^0 production out to transverse momentum of 16 GeV/c, "jet" structures at high transverse momentum, triple "jet" structures, and direct-γ production. With the closing down of the ISR, their CERN effort is now being directed towards the SPS Experiment UA-6. This experiment will use an internal hydrogen gas-jet target to study p-p and $\bar{p}$-p collisions at 270 GeV. One unique feature of the target is that it can be polarized. Apparatus is being prepared to investigate topics similar to those studied at the ISR, providing detailed comparison between proton and antiproton cross sections.

Goals and/or Major Results to Date

The ISR experiment discovered the high transverse momentum phenomenon. One of its most recent results is that the cross section for α-α production compared to p-p production of high transverse momentum π^0 mesons was found to be larger than expected by a factor of about two at the highest p_T observed. It is hoped that the new data with α-α, p-α, and d-d collisions will provide some new insights into this unexpected phenomenon.

The UA-6 experiment at the SPS will be taking its first data in the fall of 1984. It is expected that comparison of $\bar{p}$p and pp data, particularly transverse momentum distributions, will help to reveal the importance of higher order QCD diagrams.

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Title of Project: Fermilab Program

Person in Charge: K. Goulianos

Scientific and Professional Staff: S. Belforte, T. Chapin, and S. White

ROCKEFELLER UNIVERSITY
New York, New York

Scope of Work

The Fermilab program has focused on experimental studies of the diffraction excitation/dissociation of high energy hadrons and photons, $h(\gamma)+p \to X+p$. For the photon case, they developed and built a novel high-pressure hydrogen Time Projection Chamber (TPC), which served both as target and detector of the recoiling protons. Recently the group joined the Collider Detector Facility (CDF) collaboration at Fermilab with the intention of studying diffraction dissociation at collider energies. For this purpose, they will collaborate closely with the Pisa-Frascati groups of CDF in building a silicon recoil spectrometer to be installed inside the vacuum pipe of the collider. They will, of course, also participate as full members in the entire physics program of CDF.

Goals and/or Major Results to Date:

The differential cross sections for diffraction dissociation of hadrons on hydrogen are exponential in t, vary as $1/M_x^2$, exhibit factorization, and obey the Finite Mass Sum Rule (FMSR). These characteristics are typical of triple Pomeron dominance in the amplitude. Photon dissociation shows the same characteristics except that the FMSR is only obeyed if the "incident hadron" mass is taken to be the mass of the ρ-meson. This result supports the Vector Dominance Model.

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Title of Project: Neutrino Mass Measurement

Person in Charge: O. Fackler

Scientific and Professional Staff: H. Sticker

Scope of Work

This group, in collaboration with Marshall Mugge from Fermilab, and Roger White and Robert Woerner from Lawrence Livermore Laboratory, is conducting an experiment to determine the electron $\bar{\nu}$ mass by measuring the shape of the tritium β-decay energy distribution near its endpoint. The experiment is unique in its use of a large area, high-activity frozen tritium source. The use of this source enables them to make an accurate calculation of the excited final molecular state effects.

Goals and/or Major Results to Date

The experimental set-up is almost complete and spectrometer resolution studies are under way. If the tritium associated background is as low as anticipated, they expect to be able to determine the electron $\bar{\nu}$ mass to ±2 eV for a mass greater than 4 eV.

ROCKEFELLER UNIVERSITY
New York, New York

Title of Project: Theoretical High Energy Physics

Person in Charge: M. A. B. Beg

Scientific and Professional Staff: M. A. B. Beg, L. Dolan, Y.K. Ha, B. Ovrut, A. Sirlin, T. Tomaras, W. Marciano, R. Furlong, C. Panagiotakopoulos, and P. Simic

Scope of Work

The mission of participants in this program is fundamental research in theoretical high energy physics. The interests of members of the group cover a wide range of topics, from sophisticated mathematical constructs (for description of physical phenomena) to phenomenology and analysis of experiments; nonetheless, it is a coherent group held together by a commonality of outlook; all work within the framework furnished by gauge field theory, the language of modern theoretical physics, and use group-theoretic techniques, its most potent mathematical tool.

There is an active visiting scientists program. Visitors during the preceding year included Julius Wess, Edward Corrigan, Michael Duff, Sidney Drell, John Iliopoulos, and Luigi Radicati.

Goals and/or Major Results to Date

During FY 1984 members of the group were engaged, and produced important results, in the following research topics: consistency of the Salam-Weinberg theory and upper bounds on the mass of the Higgs boson, $\Delta S=2$ amplitudes, in the Technicolor/Hypercolor Scenario, applications of the infinite parameter affine Kac-Moody algebras to the non-perturbative states of Yang-Mills theory, conformal gravity, Kaluza-Klein monopoles, infra-red stability of non-Abelian gauge theories, dynamical mass generation, sigma models with U(N) gauge invariance, radiative corrections to various parameters in the standard model (in particular, precise determinations of $W^{\pm}$ and Z masses), breaking of extended supersymmetry, supersymmetry, and inflation, etc.

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Title of Project: Theory

Principal Investigator: N. N. Khuri

Scientific and Professional Staff: M. Evans, V. Figerou, B. Grossman, H. Kappen, N. N. Khuri, J. McCarthy, H. R. Pagels, and A. Sanda

ROCKEFELLER UNIVERSITY
New York, New York

Scope of Work

Members of this group work in basic theoretical physics research covering various areas of high energy physics and particle physics. In addition problems in mathematical physics of relevance to quantum field theory are investigated.

Goals and/or Major Results to Date

During FY 1984, members of this group produced important results in the following research areas: Development of a new method to obtain rearrangement inequalities in mathematical physics, new results on the Borel summability of lattice field theories, dimensional reduction of Yang-Mills theories, the problem of CP violation in nature, geometrical properties of two dimensional non-linear sigma models, and cosmological consequences of gauge field theories.

Work in the above areas continues and new paths are being explored all aimed at the ultimate goal of understanding the basic structure of matter.

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UNIVERSITY OF ROCHESTER
Rochester, New York

Award No.: DE-AC02-76ER13065

Title of Project: AMY

Persons in Charge: S. Olsen and A. Bodek

Scientific and Professional Staff: A. Bodek, S. Olsen, and T. Gentile

Scope of Work

AMY is a detector for TRISTAN, an e^+e^- storage ring under construction at KEK, the Japanese National Laboratory for High Energy Physics, which is based on a small high field solenoid magnet. The high field provides the ability to do precise momentum measurements in a small volume. For high momentum particles, the estimated precision is comparable to that of larger, more conventional detectors which particularly emphasize good momentum resolution, and for low momentum tracks is superior to any other e^+e^- device. The synchrotron x-rays emitted by final state electrons provide a clean, convenient signature which enables extremely good π/e discrimination. The small size and highly magnetized flux return iron make the detector well suited for muon detection. The entire detector is compact and readily accommodates low-beta configurations of the storage ring. By specializing the detector to those features they chose to emphasize, i.e. momentum resolution, lepton detection and γ/π^0 discrimination, they find that they can achieve state of the art levels in these areas with a device which has only a few detection systems that use well understood detector technology.

Goals and/or Major Results to Date

The TRISTAN energy region, $45 < \sqrt{s} < 70$ GeV is totally unexplored. The AMY experiment is designed to study this region with good sensitivity searching for new quark and lepton states, the elementary scalars implied by the Higgs mechanism, and possible scalar versions of the Z^0 boson. Tests of QED and the electroweak theory will be performed. If a heavy quark system is found in this energy range, the properties of the quark-antiquark potential at separation distance of .03 fermis will be studied, an order of magnitude smaller than the distances probed by the charm and bottom quark systems.

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Title of Project: Neutrino Interactions and Lepton-Hadron Processes

Person in Charge: A. Bodek

Scientific and Professional Staff: H. Budd, F. Borcherding, J. L. Ritchie, I. E. Stockdale, and K. Lang

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UNIVERSITY OF ROCHESTER
Rochester, New York

Scope of Work

The group is pursuing several fields of research. The physics emphasis of the program can be broken up into three categories.

1. Neutrino Interactions--Deep Inelastic Scattering, Charged Current Structure Functions and QCD tests, Studies of Neutral Currents, Multimuon Events and Neutrino Oscillations
2. Hadronic Production of Prompt Muons--Prompt single muons, dimuon and trimuon events are signatures of charm and bottom particle production. These leptonic final states are used to infer charm production cross sections and production mechanism in hadronic collisions. Dimuon events are used to place limits on D^0-$\bar{D}^0$ mixing and bottom particle production.
3. Deep Inelastic Scattering from Nuclear Targets--Electron scattering from nuclear targets is used as a tool of determining quark distributions in nuclei.

Goals and/or Major Results to Date

Detailed measurements of neutrino interactions have yielded information on structure functions and total cross sections. Neutrino charged and neutral current events were used to extract the Weinberg angle. Dimuon events were used to extract the strange quark sea and like sign dimuons (which are presently unexplained) were observed. Trimuon events were first discovered by this collaboration. The hadronic production of prompt muons experiment has yielded the best determination of charm production cross sections and distributions, the best limits on D meson mixing, and limits on bottom particle production. The electron scattering experiments have yielded the first confirmation of the EMC effect which is evidence for the distortion of the quark distributions inside the nucleon when it is in the presence of other nucleons in the nucleus.

The group plans to continue the study of neutrino interactions and higher values of momentum transfers using the Fermilab Tevatron neutrino beams.

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Title of Project: Theory

Person in Charge: S. Okubo

Scientific and Professional Staff: A. Das, C. R. Hagan, V. S. Mathur, and S. Okubo

UNIVERSITY OF ROCHESTER
Rochester, New York

Scope of Work

The main research activity of this group is in the area of basic high energy theoretical physics, especially in connection with symmetry principles and phenomenology of particle physics, Lagrangian field theory, mathematical physics and more recently studies of supersymmetry. Some of them are jointly working on various problems with scientists at Montreal, St. Louis, Los Alamos, and India. Also, four nearby universities--Montreal, Rochester, Syracuse, and Toronto--have been operating a joint annual regional high energy seminar for the past four years.

Goals and/or Major Results to Date

Among recent major works, they mention a successful calculation of D^+-D^0 mass difference on the basis of a QCD sprectral sum rule, a strong coupling expansion calculation of two-dimensional supersymmetric theory on a lattice, and work on existence of indecomposable representation in super-space of supersymmetry theory. With respect to mathematical physics a theory of general Dynkin indices of any simple Lie algebra has been formulated. This will help any group theoretical calculation involving Clebsch-Gordan decomposition and branching rules in high energy theory.

They are still pursuing many problems concerning supersymmetry and supergravity theory as well as a classification of general local gauge theories.

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Title of Project: A Comprehensive Study of Direct Photon Production in Hadron Induced Collisions (Fermilab E706)

Persons in Charge: T. Ferbel and P. Slattery

Scientific and Professional Staff: C. Chandlee, T. Ferbel, P. Gutierrez, J. Huston, P. Slattery, G. Ballocchi, A. Lanaro, J. Mansour, and N. Mathur

Scope of Work

The primary physics objectives of Fermilab experiment E706 are to study the gluon structure functions of hadrons and to investigate gluon fragmentation through analyzing the production of single direct photons and their accompanying hadrons in collisions of pions, kaons, and protons with a variety of nuclear targets. Th underlying constituent interactions to be investigated are: $gg \rightarrow q\gamma$ and $\bar{q}q \rightarrow g\gamma$. In addition, events containing high mass diphoton pairs will be analyzed. By studying, in a single experiment, the relative yields of $\gamma\gamma$ and e^+e^- triggered events, an essentially unbiased comparison will be made between the two fundamental quark-antiquark annihilation reactions: $qq \rightarrow \gamma\gamma$ and $\bar{q}q \rightarrow \ell^+\ell^-$. The apparatus will also be used to investigate associated jet production via triggering on the simultaneous production of pairs of high transverse momentum hadrons.

UNIVERSITY OF ROCHESTER
Rochester, New York

Goals and/or Major Results to Date

Experiment E706 has been granted second stage approval by Fermilab (in October 1983), and the present emphasis of the collaboration is on the construction of the powerful multiparticle spectrometer which will be required to achieve its experimental goals. The central element of the E706 spectrometer is to be a fine-grained liquid argon calorimeter, and this task has the shared responsibility for constructing this device (along with the NSF supported University of Rochester high energy experimental group headed by F. Lobkowicz). Progress to date has been entirely satisfactory and consistent with the presently scheduled experimental startup date of March 1986. This task also has the responsibility for coordinating the activities of the other collaborating groups; progress on the construction of the other spectrometer components is proceeding apace.

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Title of Project: Study of e^+e^- collisions with the CLEO detector at the Cornell Electron Storage Ring

Persons in Charge: S. L. Olsen and A. C. Melissinos

Scientific and Professional Staff: T. Gentile, A. Melissinos, S. Olsen, D. Peterson, S. Behrends, K. Chadwick, and G. Parkhurst

Scope of Work

The systematic study of the properties of the b-quark and of particles containing a b-quark. The Cornell Electron Storage Rings and the CLEO detector, in particular, are the best available facilities in the whole world for these studies. The group has been a part of this collaboration since it was first formed and, therefore, has in the past and continues to contribute to the extensive series of discoveries about the heavy quarks as detailed below.

Goals and/or Major Results to Date

Among the major results of this work are: 1) the precise determination of the parameters of the γ-family which consists of a $(b\bar{b})$ bound state, 2) The observation of transitions between the states of the γ-family and the discovery of the ^3P states, 3) the discovery of the B-meson and of some of its decay modes, 4) the study of the weak decay of the b-quark, and 5) the absence of flavor changing neutral currents and of other "exotic" processes, strongly supporting the existence of the (top) t-quark.

Among the immediate goals for the future are: 1) the observation of B^0-$\bar{B}^0$ mixing and possibly of CP violation in this system, 2) much more detailed studies of the b-quark decay, 3) highly improved studies of quark fragmentation, 4) precise determination of the QCD coupling constant, and 5) a renewed search for new particles as suggested by recent theoretical work.

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UNIVERSITY OF ROCHESTER
Rochester, New York

Title of Project: Search for the Gravitational Effects of a Stored Beam of High Energy Particles

Person in Charge: A. C. Melissinos

Scientific and Professional Staff: A. C. Melissinos, P. Reiner, J. Rogers, and W. Wuensch

Scope of Work

To explore the possibility of detecting the gravitational effects of a stored beam of very high energy particles. Such an experiment is, so far, the only proposed laboratory test of Einstein's theory of general relativity. In principle the energy dependence of the effect provides a measure of the spin of the graviton.

Goals and/or Major Results to Date

They have developed a superconducting microwave coupled cavity system which is suitable for the detection of high frequency gravitational perturbations. With this system they have demonstrated the measurement of harmonic displacements of order 3×10^{-19}m (in a narrow bandwidth of ~10^{-3}Hz). Their immediate goal is to search for this effect at the Fermilab accelerator and to access experimentally the background level.

Such high Q systems are also suitable for searches of particles that couple to the electromagnetic field even if very weakly. One possibility is to search for cosmic "axions" of very low mass. Finally, the technology developed for these detectors has direct applications to superconducting cavities for high energy electron accelerators.

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SAN FRANCISCO STATE UNIVERSITY
San Francisco, California

Award No.: DE-AC03-81ER40009

Title of Project: Search for Stable Quarks

Persons in Charge: R. W. Bland and C. L. Hodges

Scientific and Professional Staff: R. Bland, C. Hodges, R. Johnson, D. Joyce, M. Lindgren, M. Savage, and B. Young

Scope of Work

This group's primary activity is the search for free fractionally charged particles (quarks). The group has developed an automated version of the Millikan oil drop experiment. The group searches for free quarks in natural materials and for free quarks produced in targets exposed to high energy particle beams.

Goals and/or Major Results to Date

The major results from this group have been a search in 1981 for free quarks in native mercury, a search during 1983 for free quarks in natural waters, and a search during 1983 for free quarks produced in material exposed to a heavy ion beam at the Bevalac. There was no evidence in any of the three searches for free quarks.

The goals of the group are to measure a much larger sample of materials and to try various methods of concentrating quarks. They are developing a modification of the Bevalac experiment to be used at Fermilab. Finally, the group is working on an apparatus that would use continuous streams of drops with vertical rather than horizontal electronic deflections.

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SMITHSONIAN INSTITUTION
Amado, Arizona

Award No.: DE-AC02-82ER40063

Title of Project: Very High Energy Gamma Ray Astronomy

Person in Charge: T. C. Weekes

Scientific and Professional Staff: K. Gibbs

Scope of Work

High energy gamma ray astronomy provides a direct link to high energy particle activity in cosmic sources; it is the most direct means of locating the sources of cosmic radiation.

To improve the flux sensitivity of the atmospheric Cerenkov technique in very high energy (100 GeV - 10 TeV) gamma ray astronomy, the 10 m optical reflector on Mount Hopkins in southern Arizona is being converted to a very fast, large aperture, low resolution camera. The image of each Cerenkov light "spot" is recorded digitally to give improved angular resolution. The use of a narrow-beam trigger permits extension of the technique to energies < 100 GeV; operation at large zenith angles gives sensitivity to gamma rays of energy > 10 TeV. The completed camera should have a flux sensitivity a factor of ten better than previous experiments at 1 TeV. It will be used to study all known or potential sources in the Northern Hemisphere.

Goals and/or Major Results to Date

The gamma ray imaging technique has been developed and more than one million images from candidate sources detected. In preliminary observations fluxes were detected from Cygnus X-3 and the Crab pulsar. The device was also used to set limits to the flux of low velocity monopoles (assuming the Rubakov effect). The current observing program includes the newly discovered millisecond pulsars, X-ray binaries, the 100 MeV gamma ray sources and extragalactic objects; many of these may also be sources of high energy neutrinos.

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1113

UNIVERSITY OF SOUTH CAROLINA
Columbia, South Carolina

Award No.: DE-AC09-80ER10690

Title of Project: Electron--Positron Annihilation

Person in Charge: C. Darden

Scientific and Professional Staff: R. Childers, H. Gennow, and T. Phan

Scope of Work

This group consists of four experimental physicists doing fundamental research in the area of particle physics. It is part of a larger group, the ARGUS collaboration, studying electron-positron annihilation at energies from about 9.5 to 11.5 GeV. Upsilon mesons which are bound states $b\bar{b}$ of the b quarks are produced in this energy range.

The ground state (1S) or any of the five known excited states are produced when the energy of the storage ring matches the energy of that state. They study the decay modes of a state by detecting the particles produced when it decays, measuring their velocity, specific ionization, momentum, charge, or in the case of photons, their energy.

Interest in Upsilon mesons is particularly high because relatively little is known about them. They were only discovered in 1978.

The group completed its first year of data taking in December 1983 after spending nearly four years designing and building a suitable detector.

The detector has an 8000 gauss solenoidal magnetic field, a drift chamber with 5940 sense wires, 160 time-of-flight scintillation counter, an electromagnetic shower calorimeter with 1760 lead-scintillator stacks, and a muon identification system consisting of 1744 tube chambers behind a layer of iron.

Goals and/or Major Results to Date

The main accomplishment of the group in 1982 was getting this complex detector working. It was a sizable job that included an enormous amount of computer programming. In 1983 they took data. The results for the year include a precise determination of the mass of the Upsilon 2S which was made jointly with the Crystal Ball collaboration and the DESY polarization group, the discovery of a new decay mode for the F meson, confirmation of the mass of the F meson reported by the CLEO collaboration, and a beautiful, precise spectrum for the photons in the electromagnetic transition $\Upsilon(2S) \rightarrow \Upsilon(1^3P_J)$, confirming these three lines reported earlier by the CUSB collaboration.

Goals for the future include understanding the decays of the B mesons. These mesons are produced when the $\Upsilon(4S)$ decays. They contain one b quark and a lighter anti-quark.

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1114

UNIVERSITY OF SOUTHERN CALIFORNIA
Los Angeles, California

Award No.: DE-AC03-84ER40168

Title of Project: Preons, Supersymmetry, Non-Perturbative Field Theory

Person in Charge: Bars

Scientific and Professional Staff: Bars

Scope of Work; Goals and/or Major Results to Date

Research is proposed on three broad subjects in fundamental theories in particle physics:

1. Composite Quarks and Leptons,
2. Supergravity and Nuclear Supersymmetry, and
3. Non-perturbative Methods in Gauge Theories

Methods to be employed include fundamental tools of quantum field theory, group theory, and supersymmetry. This research is directed to some of the basic problems presented by the current theoretical and experimental status of particle physics. By studying compositeness they explore the possible physics beyond the boundaries of the "standard model" starting at energies of 1 TeV or above, appropriate to the next generation of accelerators currently under construction or consideration. They analyze the geometrical structure of supergravity to explore the possibility of an ultimate unification of forces including gravity. At low energies, they try to understand the dynamical origin of effective supersymmetries in nuclei that are phenomenologically successful. By studying non-perturbative methods in field theory, they hope to provide new insights for solving QCD as well as some of the new theories of composite quarks and leptons. They expect that these topics will continue to be of fundamental significance in the advancement of high energy physics in the coming few years.

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STANFORD UNIVERSITY
Stanford, California

Award No.: DE-AT03-82ER40076

Title of Project: Superconductive Monopole Detectors

Person in Charge: B. Cabrera

Scientific and Professional Staff: J. Bourg, R. Gardner, M. Huber, and M. Taber

Scope of Work

Grand Unification Theories have revived the search for magnetic monopoles by predicting the existence of supermassive particles carrying the Dirac magnetic charge. Such massive particles would be relics from the early universe and would not be captured in matter. Thus searches in the cosmic rays are required. Superconductive detectors directly measure magnetic charge independent of other particle properties, and the detector sensitivities are based on simple fundamental principles.

Goals and/or Major Results to Date

The goal is to optimize the design, both in cost and detection efficiency, of a superconductive detector with a sensing area of at least 100 m^2 times 4π steradians. They have set a particle flux limit of 1.1×10^{-11} cm^{-2} sec^{-1} sr^{-1} (90 percent C.L.) using a three loop detector which has operated continuously for over a year. This flux limit is over 100 times lower than that suggested by the single event on the single loop prototype detector. They are now building a new detector with 30 times the sensing area of their present detector (1.5 m^2 times 4π sr) which they view as a prototype for the 100 $m^2 \times 4\pi$ sr future array.

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1116

STANFORD UNIVERSITY
Stanford, California

Award No.: DE-AT03-76ER71042

Title of Project: Laser-Driven Particle Accelerators

Person in Charge: R. H. Pantell

Scientific and Professional Staff: M. A. Piestrup, A. M. Fauchet, and D. Y. Wang

Scope of Work

The purpose of this program is to investigate particle acceleration by means of laser light. The advantage to the use of lasers for acceleration is that high field strengths can be achieved, thereby allowing for high acceleration gradients. The group is interested in exploring a number of methods for achieving this interaction including the inverse Cerenkov effect, two wave interaction, and the gas loaded inverse free-electron laser.

Goals and/or Major Results to Date

The group has successfully momentum-modulated a 102 MeV electron beam using a 30-MW Nd:YAG 1.06-μm laser beam. The interaction occurred within the gas which retards the phase velocity of the light wave in order to allow wave vector matching with the electron velocity. The maximum amount of energy exchange was approximately 200 keV.

Another experiment was also done wherein coherent Cerenkov radiation at 0.532μm was observed from an optically bunched electron beam. Bunching was induced by means of the inverse Cerenkov effect. The pressure dependence of this radiation was verified.

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1117

SUPERCON, INC.
Natick, Massachusetts

Award No.: DE-AC01-81ER40044

Title of Project: Development of High Field Superconductors for High Energy Particle Physics

Person in Charge: J. Wong

Scientific and Professional Staff: E. Gregory, R. N. Randall, and W. L. Larson

Scope of Work

The objective is the development of a high current composite superconductor for use in high energy accelerator magnets operating at fields above 10 Tesla. The composite conductor will consist of a high conductivity copper matrix containing tubular niobium filaments with cores of tin or a high tin-copper alloy. In developing the conductor design and in testing various fabrication techniques several variables will be examined; these include the copper to filament ratio, the niobium to tin ratio in the filament, the relative niobium-tin interfacial area, the behavior during deformation of the high tin-copper alloys when in a composite with niobium and copper, and the use of swagging, drawing, and extrusion. A manufacturing procedure for long lengths of conductor will be subsequently developed and refined. Concurrently, the necessary quality assurance tests and inspections will be developed and possible inspection equipment evaluated.

Goals and/or Major Results to Date

The goal is the production of 150 pounds of composite conductor of a size of interest to the accelerator magnet designers at the Department of Energy national laboratories. This conductor is to be produced as production material rather than under laboratory conditions. The wire is to be inspected and tested so that its pertinent construction and performance characteristics can be fully described.

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1118

SYRACUSE UNIVERSITY
Syracuse, New York

Award No.: DE-AC02-76ER03533

Title of Project: Research Program in Elementary Particle Theory

Person in Charge: K. C. Wali

Scientific and Professional Staff: A. P. Balachandran, H. Gomm, O. Kaymakcalan, C. Rosenzweig, and J. Schechter

Scope of Work

Although the group at Syracuse is relatively small, its interests are wide. Areas of research range from phenomenological studies to purely formal considerations. Permanent members, or visitors, have recently been active in phenomenology of proton decay, grand unified theories, glueball physics, topological issues in field theory, monopoles, soliton models for baryons, axions, neutrino masses and oscillations, effective Lagrangians, supersymmetry, QCD, and confinement. They participate regularly in national and international conferences and have an active seminar schedule with invited speakers from all over the U.S. They frequently have visitors from other nations stay with them from periods of a few weeks up to one year.

Goals and/or Major Results to Date

They are proud of the fact that members of the Syracuse group have been responsible in major ways for the revival of soliton models for baryons, for the modern incarnation of effective Lagrangians in QCD and supersymmetry, and for study of the generation problem in GUTs. They expect to continue their activities and contributions to major areas of particle physics research. They are particularly proud of the quality of their Ph.D. students in recent years.

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1119

UNIVERSITY OF TENNESSEE
Knoxville, Tennessee

Award No.: DE-AS05-76ER03956

Title of Project: Experimental Elementary Particle Physics

Person in Charge: W. M. Bugg

Scientific and Professional Staff: J. E. Brau, G. T. Condo, T. Handler, J. Hargis, and E. L. Hart

Scope of Work

The contributions of this group to the advancement of elementary particle physics has been primarily in the area of hybrid-bubble chamber experiments. The present analysis effort is concentrated in two experiments which have completed data taking. The first is the charm photoproduction experiment at SLAC (BC 72, 73, 75, 76) while the other, (Fermilab 565-570), is a study of the high energy interaction of $(\pi^+ K^+, p)$ with hydrogen and thin metallic plates (Ag, Au) placed in the bubble chamber. Both of these experiments have, as their principal feature, downstream particle identification in conjunction with high resolution detection of the interaction vertex. In both experiments significant contributions to the experimental hardware and software have been made by this group. They have also been principals in certain aspects of the data analysis for the SLAC experiment. The Fermilab experiment is just entering the data analysis phase.

A smaller, local effort is under way to search for the neutral, $S = -2$, stable, dibaryon, predicted by the MIT bag model, from slow $\bar{p}$ annihilations in complex nuclei.

The group is preparing for studies of neutrino interactions at Tevatron energies in the Tohoko Holographic Bubble Chamber. These studies will be highlighted by a search for τ neutrino interactions in the Fermilab beam dump facility. Tennessee is constructing the drift chambers for these experiments.

They have also joined the SLD collaboration at SLC and are currently working on the calorimeter and the luminosity monitor. A major portion of future effort will be devoted to this project.

Goals and/or Major Results to Date

The principal results to date from the SLAC experiment include measurements of the open charm photoproduction cross section at 20 GeV/c laboratory momentum and the lifetimes of D^0 and $D^\pm$ mesons. While the measured lifetime of the charged D is compatible with that obtained in other experiments, their value for the D^0 lifetime exceeds that reported by other investigators by more than a standard deviation. An offshoot of

UNIVERSITY OF TENNESSEE
Knoxville, Tennessee

this experiment was recently completed, where a search for the reaction, $\gamma p \to D^{-}\Sigma^{+}{}_{c}{}^{+}$, was made approximately 700 MeV above threshold. This experiment, which produced a null result, was predicated on the suggestion that the "contact term" in the electromagnetic Lagrangian, which explains, e.g., the large cross section observed for the reaction $\gamma p \to \Delta^{++}\pi^{-}$ near threshold, would strongly enhance the $D^{-}\Sigma^{+}{}_{c}{}^{+}$, final state.

Data analysis from Fermilab E-565-570 has as yet produced only information on charge excess from hadronic collisions with light and heavy nuclei. A positive particle excess has been shown to persist up to high momenta.

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UNIVERSITY OF TEXAS
Austin, Texas

Award No.:	DE-AS05-76ER03992
Title of Project:	Research Program in Elementary Particle Theory
Persons in Charge:	E. C. G. Sudarshan and D. A. Dicus

Scientific and Professional Staff: A. Bohm, C. B. Chiu, D. A. Dicus, A. M. Gleeson, Y. Ne'eman, E.C.G. Sudarshan, A. Stern, and S. Nandi.

Scope of Work

Members of the Center for Particle Theory at the University of Texas do basic research in theoretical physics. The emphasis is on high energy physics but work is also done in the areas of quantum optics, medium energy physics, astrophysics, and cosmology. In particular, these areas are used as additional testing grounds for the current ideas of high energy physics.

Most of the work done at the Center involves the active participation of graduate students. In addition, the Center has many visitors each year whose stay lasts from a week to all year. Every attempt is made to draw these visitors into ongoing collaborations or to start new interactions.

Goals and/or Major Results to Date

During FY 1983, important results were produced in the following areas: topology of magnetic monopoles; spontaneously broken supersymmetry; supersymmetry at finite temperature; lepton number violation in stellar collapse; pion condensation in neutron star matter; W decay in supergravity GUTS; Wino decay from $\bar{p}p$; e^+e^- annihilation cross-section in supergravity; fits to hyperon decay data; paraxial wave optics; first order optical systems; etc.

Almost all of these topics continue to be of interest with particular emphasis on the Lorentz invariance of monopoles, the phenomenology of supersymmetry, and finite temperature field theory.

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TEXAS A&M UNIVERSITY
College Station, Texas

Award No.: DE-AS05-81ER40039

Title of Project: High Energy Physics Research

Persons in Charge: R. C. Webb and P. M. McIntyre

Scientific and Professional Staff: T. Meyer, P. M. McIntyre, R. C. Webb, A. David, and N. Diaczenko

Scope of Work

This group is primarily involved with research in experimental high energy physics using counter and chamber techniques. At present, they are participating in two separate research projects. The first of these experiments is a search for super heavy GUT magnetic monopoles in cosmic rays. This experiment utilizes a large area scintillation counter array which has been assembled underground in a nearby salt mine. They are just beginning to take data with this detector. The second experiment in which they are involved is the Colliding Detector Facility (CDF) at the Fermilab $\bar{p}p$ collider. This group is constructing the forward/backward hadron calorimeter systems for this detector facility. They expect the first data taking runs with the completed detector will be sometime in 1986. This detector will be used to investigate the details of hadron collision at c-m energies of nearly 2 TeV. The CDF program is expected to continue for several years once data taking begins.

Goals and/or Major Results to Date

The present goal for the monopole search is to investigate the flux of monopoles in a relatively unexplored region of phase space (velocity). The spectrometer has good efficiency for detecting monopoles with velocities in the range $5 \times 10^{-4} < \beta < 10^{-2}$. In one year of data taking they will be able to establish a flux list of $10^{-14}\text{cm}^{-2}\text{sr}^{-1}$.

The goals for the CDF project are to investigate in detail the properties of very high energy hadron collision. The detector is capable of studying in detail the following processes: high transverse momentum phenomena, QCD jets, $W^{\pm}$ and Z^{0} decays and asymmetries, heavy flavor production, and other oddities like centauro events.

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1123

TUFTS UNIVERSITY
Medford, Massachusetts

Award No.: DE-AC02-83ER40085

Title of Project: High Energy Physics at Tufts University

Persons in Charge: R. H. Milburn and J. Schneps

Scientific and Professional Staff: G. R. Goldstein, T. Kafka, W. A. Mann, R. H. Milburn, A. Napier, W. P. Oliver, J. Schneps, and R. K. Thornton

Scope of Work

The Tufts group continues collaborative investigation probing the mechanisms of production, interaction, and decay of the elementary constituents of matter. Recent examples include studies of neutrino interactions in deuterium as observed in the Fermilab 15-ft bubble chamber, of $K_S^0 K_S^0$ and $\phi\phi$ production at the Fermilab MPS, of vector-meson photoproduction and lifetime measurements of charmed particles in the SLAC Hybrid Facility, of ϕ and K^{0*} production based upon SLAC Streamer Chamber data, and of hadronic production of χ mesons at Fermilab. A study of neutrino interactions in the 15-ft chamber will commence shortly at the Fermilab Tevatron.

The group also is part of the Soudan II nucleon decay project, based upon a 1200-ton fine-grained iron calorimeter to be installed in Minnesota. This experiment will provide improved limits on the nucleon lifetime, especially with respect to decays into complex multiparticle final states not easily resolvable by the water-Cerenkov technique, and it will have an enhanced ability to reject neutrino background events to facilitate the observation of any nucleon decays which may occur.

Theoretical investigations include studies of diquark-quark baryon models, of the general kinematic description of scattering processes, and of QCD radiative corrections to hadron potentials.

Goals and/or Major Results to Date

Accomplishments include: a first determination of the charmed baryon component to inclusive Λ^0 production in charged-current reactions and a variety of data on neutrino total cross sections into charged-currents, charged-current multiplicities from n and p, and the mass parameter of the axial vector form factor; also new results from direct measurements of the lifetimes for decay of charged and neutral charmed particles; also results on the mechanism of hadronic J/ψ production, on conjoint-ϕ production, and on systems containing multiple strange quarks. In theoretical work an optimal representation of two-body scattering processes, including polarization dependence, has been developed.

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1124

UNIVERSITY OF VIRGINIA
Charlottesville, Virginia

Award No.: DE-FG05-84ER40157

Title of Project: Symmetry Principles In Particle Physics

Person in Charge: P. K. Kabir

Scientific and Professional Staff: P. K. Kabir

Scope of Work; Goals and/or Major Results to Date

Continuing interest in CP violation and presumably related T noninvariance has been applied in two different ways. First, tests of T invariance, with and without associated parity nonconservation, have been proposed using polarized neutrons. These are encouraged by the unexpectedly large parity nonconserving effects found in slow neutron optics. Second, the results of improved measurements on the 2π decay amplitude ratios for K_L and K_S mesons, which failed to detect any difference between charged and neutral modes, together with data on charmed and b decay rates, encourage a reanalysis of CP violation in K^0 decays. In particular, it is intended to try to answer the question whether generalized Cabibbo (Kobayashi-Maskawa) mixings suffice to account for the observed magnitude of the CP violation parameter ϵ.

Other investigations related to the question of possible baryon-nonconserving n-$\bar{n}$ transitions. It was noted by Glashow that, even if such transitions are possible for free neutrons, the earth's magnetic field would strongly suppress them. Two alternative schemes were proposed to remove this inhibition, even without requiring exclusion of the terrestrial magnetic field.

An apparently unrelated investigation, whose results are under analysis, is a gravity experiment. Theories which attempt to unify gravity with other interactions, based on spontaneously broken supersymmetry, encourage a search for short range forces associated with ordinary gravity. Therefore, a search was made for possible deviations from Newtonian gravity in the range 10-100 m, which could be as large as 10 percent on the basis of existing knowledge. The present experiment should be sensitive to any deviation exceeding 1 percent in this range.

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VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY
Blacksburg Virginia

Award No.: DE-AS05-80ER10713

Title of Project: Electron-Positron Interactions

Person in Charge: A. Abashian

Scientific and Professional Staff: A. Abashian, K. Gotow, S. Schnetzer, F. Kajino, R. Jones, and J. Miller

Scope of Work

This group is part of the AMY collaboration which has been approved by the National Laboratory for High Energy Physics in Japan to conduct studies of the interaction of high energy electrons and positrons at the TRISTAN collider currently under construction and due to be operational in 1986. The responsibility of the VPI group is the development and construction of that portion of the AMY detector dealing with the measurement of electromagnetic showers produced in those interactions. This includes the construction of a 15 ton cylindrical detector segmented into many alternate layers of proportional tube and lead.

Goals and/or Major Results to Date

Activity in this area has been going on largely for the past several months and has emphasized the design of the detector and the development of techniques and procedures for fabricating and assembling the detector together. Prototypes have been and are continuing to be developed. Special fixtures and jigs for making panels have been designed and are in the process of being built.

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Title of Project: Theory of Weak Interactions and Related Topics

Person in Charge: R. E. Marshak

Scientific and Professional Staff: Y. Tosa, G. Branco, J. Gipson, J. Pasupathy, G. Senjanovic, Y. Okamoto, and P. Wang

Scope of Work

Research in particle theory under this contract has been carried out in five areas: 1) extensions of the standard electroweak model that relate parity breaking to the breaking of B-L local symmetry (B and L are the baryon and lepton numbers); 2) possible detection of neutron oscillations (in contrast to proton decay) in various types of unification models;

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Blacksburg, Virginia

this process requires an intermediate mass scale of the order of 10-100 TeV; 3) basic differences between the SU(5) and SO(10) grand unification groups, with emphasis on the attractive features of SO(10) from both a mathematical and physical point of view; 4) development of a three-fermion gauged preon model that could, under plausible conditions on the confining metacolor group and on the color-flavor group, explain the existence of the three generations of quark and lepton doublets; and 5) study of topologically interesting properties of gauge theory such as the possible existence of quasi-stable Higgs solitons and the role of chiral anomalies in higher dimensions. In addition to the research program, this contract has helped to support workshops on particle physics topics of great current interest to both theorists and experimentalists.

Goals and/or Major Results to Date

Major results to date are: 1) the demonstration that the treatment of B-L as a local symmetry has important consequences for model building in the unification of the weak, electromagnetic and strong interactions; 2) that there may be a deep connection between the breakdown of B-L local symmetry and the breakdown of parity; 3) that neutron oscillations have to be considered a serious alternative to proton decay as a baryon number violating test of unification models; and 4) that it is possible to develop a three-fermion preon model of quarks, leptons, and Higgs bosons with the correct color-flavor quantum numbers.

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1127

WASHINGTON UNIVERSITY
St. Louis, Missouri

Award No.: DE-AC02-78ER04915

Title of Project: Theoretical Physics

Person in Charge: J. E. Shrauner

Scientific and Professional Staff: C. M. Bender, J. E. Mandula, J. E. Shrauner, and N. Papanicolaou

Scope of Work

A program of research in theoretical and mathematical physics is pursued under this project. Topics of current interest include: lattice gauge theory calculations; large-order and strong-coupling perturbation theories in quantum field theory; chiral-symmetry breaking and quark condensation in QCD; classical condensates in finite-temperature field theory; and effective potentials and 1/N expansions in quantum field theory. A vigorous program of collaborations and visiting researchers thrives.

Goals and/or Major Results to Date

Important results in all of the research areas listed above have been accomplished and characterize the continuing vitality of this research program.

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UNIVERSITY OF WASHINGTON
Seattle, Washington

Award No.: DE-AC06-76ER01388

Title of Project : Experimental and Theoretical Nuclear Physics

Persons in Charge: J. J. Lord, T. H. Burnett, and R. J. Wilkes

Scientific and Professional Staff: J. Iwai, S. Krzywdzinski, S Neddermeyer, S. Strausz, and S. Sugita

Scope of Work

This group is engaged in a research program in high energy experimental particle physics using primarily nuclear emulsion techniques. They are participating in a joint US/Japan program (Project JACEE) to study nuclear interactions at energies two orders of magnitude greater than those of existing accelerators. The data are being collected with balloon-borne emulsion chambers. In addition, they will continue their ongoing program to study hadronic interactions in metal-powder loaded emulsions exposed to high energy accelerator beams. These experiments will be carried out at Tevatron energies with targets ranging from Z=13 to 74 and possibly Z=91.

They are also participants in a Fermilab experiment investigating leptoproduction on nuclei. The proposed experiment (E-665, T. Kirk, spokesman) has been approved as one of the first users of the Tevatron 750 GeV muon beam. During the coming year, the Washington contribution to the collaborative effort will involve the construction and testing of counter systems for the spectrometer and the planning of film analysis facilities and procedures.

Goals and/or Major Results to Date

The properties of nuclear interactions at high energies will reveal whether novel production mechanisms come into play due to the high nuclear densities and temperatures obtained. The primary objectives of this program are to determine the existence and properties of the hypothesized quark-gluon phase of matter. In addition, certain features of the hadronic interaction process, such as nuclear fragment production, can be observed only with emulsion techniques.

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Title of Project: Particle Theory

Person in Charge: D. G. Boulware

Scientific and Professional Staff: R. Abbott, M. Baker, S. Barr, D. Boulware, L. Brown, S. Ellis, L. McLerran, Y-S. Wu, and A. Zee

UNIVERSITY OF WASHINGTON
Seattle, Washington

Scope of Work

The particle theory group at the University of Washington is engaged in research in a variety of areas of quantum field theory and elementary particle physics. Members of the group consult with experimental colleagues on experimental questions. Periodically, a Summer Institute in Theoretical Physics is held during which theorists from a variety of institutions gather to study a topic of current interest.

There is a continuing program of work on theoretical aspects of the trapped single electron experiment of H. Dehmelt and collaborators.

In addition to engaging in theoretical research, various members of the group serve on national panels.

Goals and/or Major Result to Date

Recently, members of the group have made significant contributions in the fields of perturbative quantum chromodynamics, grand unified theories, confinement in quantum chromodynamics, quantum gravity, and atomic physics. In the fields of quantum chromodynamics, energy correlation functions and their relation to experiment were studied and, separately, the confinement mechanism is under continuing investigation. The properties and problems of higher derivative gravity theories especially the induced gravity theory, have been the focus of a great deal of activity along with work on Kaluza-Klein theories and early cosmology.

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WAYNE STATE UNIVERSITY
Detroit, Michigan

Award No.: DE-AC02-76ER02302

Title of Project: Quantum Theory of Fields

Person in Charge: S. N. Gupta

Scientific and Professional Staff: S. N. Gupta, S. F. Radford, and W. B. Rolnick

Scope of Work

This research program deals with the development of basic theories of strong, weak, electromagnetic, and gravitational interactions as well as their applications to fundamental physical processes. They are also actively collaborating with Gordon Kane of the University of Michigan and Wayne Repko of Michigan State University with frequent visits and exchange of ideas. At present, emphasis is on investigation of problems in quantum chromodynamics and supersymmetric theories.

Goals and/or Major Results to Date

Wayne State University has become a center of theoretical research in quantum chromodynamics and quarkonium spectroscopy, and recent experimental results at the Cornell Electron Storage Ring on $b\bar{b}$ spectroscopy have been found to be in excellent agreement with their predictions. Further work on quarkonium spectroscopy and other fundamental problems such as quark confinement mechanism is in progress. In addition, they are engaged in research on supersymmetric theories and their experimental implications as well as limitations placed by existing experimental results upon masses and other parameters in these theories.

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1131

UNIVERSITY OF WISCONSIN
Madison, Wisconsin

Award No.: DE-AC02-76ER00881

Title of Project: Test of Grand Unification Forces and Baryon Number Changing Processes

Person in Charge: D. B. Cline

Scientific and Professional Staff: R. Loveless, R. March, R. Morse, and T. Smart

Scope of Work

This task is concerned with experimental tests of the possible grand unification of forces which postulates that the weak, electromagnetic, and strong forces are a manifestation of a single underlying force. The two most likely tests of this concept are the nonconservation of baryon number and the existence of very massive magnetic monopoles. For the search for proton decay they have constructed and are operating a large detector (the Harard-Purdue-Wisconsin Detector) at Park City, Utah. This detector is currently operating at high efficiency and being used to search for a broad class of possible proton decay modes and employs a volume array of photomultiplier and a very large PWC active shield.

The search for magnetic monopoles at a very small concentration can be carried out using the probable trapping of these monopoles in very old iron ores. They have designed a detector to search for the monopoles being released from the ore having been heated above the Curie temperature at large industrial plants. The detector is partially completed.

They are carrying out a conceptual design of two other possible proton decay detectors: (1) A 100,000 fresh water Cherenkov detector located in a thin tank that is submerged to a depth of 5 Km in the deep ocean, and (2) A (1000-2000) ton liquid Argon detector that gives bubble chamber quality tracking. This detector could be located at the Park City site. During the next two years the search for proton decay in the various detectors in the world should lead them to decide which detector is needed for the future.

Goals and/or Major Results to Date

The goals of this research are to obtain experimental evidence for the grand unification of forces. The search for proton decay is in progress using the HPW detector at Park City, Utah. They have concentrated on decay modes that give π^+ or $\mu^\pm$ decays. One candidate has been observed. The detector is working very well at present. They are also searching for very low energy cosmic neutrinos ~30 MeV that could come from a variety of cosmological sources. The detector is unique with a volume array of PMT's and a very large gas PWC active shield around the outside. The trigger threshold is about 10 MeV.

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Madison, Wisconsin

The detector for the search for magnetic monopoles in old iron ores has been partially funded but without additional funds will not be completed.

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Title of Project: Study of Ultra High Antiproton-Proton Energy Collisions

Person in Charge: D. B. Cline

Scientific and Professional Staff: R. Handler, S. Lazic, R. Loveless, T. Markiewicz, L. Pondrom, J. Rhoades, and M. Sheaff

Scope of Work

Participants in this group pursue the study of fundamenal processes at ultrahigh energy colliders and participate in accelerator R&D to help develop ultrahigh energy colliders and detectors. This follows their initial suggestion of the $\bar{p}p$ colliders for CERN and FNAL along with Rubbia and McIntyre in 1976. Their collider program is being carried out at the CERN $\bar{p}p$ collider and the TeV I $\bar{p}p$ collider at Fermilab. The accelerator R&D is carried out in conjunction with the FNAL antiproton source group.

The major experimental effort is to study weak interactions at the energies required to produce and study the W and Z particles and to search for new particles produced in the decay of the W and Z particles such as new heavy leptons, the t quark, and a massive Higgs boson.

The effort at CERN is largely concerned with the detection of muons from fundamental processes, and they are constructing the magnetized iron wall spectrometer in conjunction with other UA1 collaborators. This detector will be crucial to the search for the t quark.

The effort at FNAL is also concerned with muon and other particle detection in the forward and angular region (1^{o}-55^{o}). Many important processes are expected to be produced in this angular region at 2000 GeV center-of-mass energy. This group, in association with the Physical Sciences Laboratory, is constructing the large magnetized toroids and tracking devices for this effort.

They are active in the development of a high energy electron cooling device using a $\sim$5 amp-4 MeV electron beam for use in a final cooldown of the antiprotons in the FNAL $\bar{p}$ source. They hope this may allow a high luminosity option for the $\bar{p}p$ collider of $L > 10^{31}$ cm^{-2}sec^{-1}. They believe this system may be useful for future antiproton colliders. They are also studying the beat wave plasma accelerator concept and there are two Ph.D. students in this program.

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Goals and/or Major Results to Date

The goal is simply to probe nature at the smallest distances with ultra high energy collisions. They have participated in the discovery of the W and Z at CERN and have helped establish the existence of QCD jets at these energies. They have helped identify the decay of the W into the $\mu + \nu$ channel and have proposed several techniques to discover the t quark and a new heavy lepton (L) (along with C. Rubbia). This work is being applied to their effort at FNAL as well.

Recently they helped discover a new class of dilepton events in the UA1 experiment with same sign leptons. These events have unusual properties that may be related to the same-sign dimuon events observed by the group in the HPW neutrino experiment many years ago at FNAL.

They have helped develop the Lithium lens system for the $\bar{p}$ sources at CERN and FNAL that promises intense antiproton collection. They have developed the concept of intermediate energy electron cooling and have measured the emittance of a high energy electron beam leading to the acceptance of the proposal of the NEC Corporation to construct an intense electron beam for electron cooling.

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Title of Project: DUMAND

Person in Charge: R. H. March

Scientific and Professional Staff: U. Camerini, M. Jaworski, J. Matthews, and R. Morse

Scope of Work

The goal of project DUMAND is to install a large phototube array on the ocean bottom to serve as a Cherenkov detector for muons and neutrinos in the TeV energy range. The project is currently in "Stage I," which calls for the deployment of seven phototubes at the chosen site, an ocean basin 30 km west of the island of Hawaii. The purpose is to test technology to be employed in the complete array and to demonstrate the scientific capabilities of the device in situ. Wisconsin shares with Purdue University the responsibility for the out-of-sea elements of the system and provides personnel as needed in Hawaii for testing, assembly, and deployment.

Goals and/or Major Results to Date

Design of all out-of-sea elements has been completed, and they are awaiting the delivery of components to complete fabrication and testing. The system will be connected to the seven-tube array via a fiber optic high speed data link. Data will be harvested by a LSI 11/73 minicomputer via a CAMAC interface, under the control of triggers provided by a parallel processor designed by M. Jaworski. Initial deployment of this system will be from an oceanographic research vessel, using a 5km cable designed to DUMAND specifications and provided on loan from the U. S. Navy. This exercise is anticipated for the spring or early summer of 1985. In the meantime, tests of undersea hardware and studies of conditions at the site are in progress, and they anticipate some participation in this effort by Wisconsin personnel resident in Hawaii.

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Title of Project: Study of Weak Interactions Induced by Neutrinos

Person in Charge: D. D. Reeder

Scientific and Professional Staff: U. Camerini, M. Duffy, W. Fry, D. Gee, R. Loveless, and M. Procario

Scope of Work

The investigators on this task have been involved for more than a decade in the investigation of the physics of the strong and weak interactions using neutrinos. In the interactions of ν's in neon hydrogen bubble chambers at Fermilab and CERN aspects of heavy quark production and decay, the weak neutral current, and lepton flavor independence of the weak interaction are being studied. A series of investigations at Fermilab using counter techniques has also contributed to the knowledge of these topics as well as charm production in hadronic interactions, which they study using the ν's from charm decay.

Among the questions still unresolved in the Weinberg Salam model of the Weak-EM interaction are: the spectrum of ν masses and the question of mixing in the lepton sector. Several experiments are being pursued to search for heavy unstable neutrinos. A new experimental technique is to be used to measure the mass of the $\bar{\nu}_e$ by measuring the end point of the tritium beta spectrum at high resolution. At CERN the collaboration is performing the last experiment using BEBC; a search for ν_μ-ν_e oscillation (appearance) using a low energy proton beam from the PS. Work is planned or in progress on the development of new techniques for the SSC era and for a new detector to be used at the projected new collider at HERA.

Goals and/or Major Results to Date

Among the more recent results obtained are: a high energy, high statistics study of ν_e interactions; the first evidence for open charm produced via the weak neutral current; a negative search for supersymmetric

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particles; observation of the A dependence of hadronic charm production; the measurement of the energy and P_t dependence of the flux of prompt ν produced in hadronic collisions; and the study of QCD effects in hadrons produced in ν interactions. They expect to identify the ν_e mass if it exists and is greater than 20 eV. The limit on ν oscillation will be the best to date using a ν_μ beam.

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Title of Project: Study of Hadronic Structure Using Hadron Induced Final States

Person in Charge: A. Erwin

Scientific and Professional Staff: M. Thompson, A. Hasan, C. Kuehn, and K. Nelson

Scope of Work; Goals and/or Major Results to Date

In 1984 this group completed a fixed target experiment at FNAL using a low magnetic field spectrometer with a towered hadron calorimeter which was designed to study jets. By laboratory fiat the experiment was limited to beam energies less than 400 GeV. Some preliminary results are as follows. (1) Single jet production cross sections multiplied by $P_T^{5.6}$ and plotted vs. x_T lie on the same curves as European jet data with cms energies 20 times higher. This scaling indicates they are looking at the same basic physics process. (2) There is a clear signal in the π-p production of high P_T events for the Berger-Brodsky process where the pion is completely absorbed and all the beam energy goes into two jets. There is no similar signal in p-p scattering. This is strong evidence for higher twist processes. (3) Double jet invariant cross sections for $d^2 \sigma/dp_T^{2y} dy_1 dy_2$ obtained with two very different triggers agree quite well with QCD predictions for this energy. (4) Data from a large number of nuclear targets show a correlation between the value of α and event planarity when cross sections are fit to A^α. The correlation is such as to indicate that higher planarity events "see" only one nucleon in the nucleus.

The group is now beginning construction on drift chambers for a small experiment in the CO intersection of TeV p-$\bar{p}$ collider. This experiment has been approved to look for evidence of a quark-gluon plasma phase of nuclear matter by studying high multiplicity events.

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Title of Project: Theoretical High Energy Physics

Person in Charge: L. Durand

Scientific and Professional Staff: A. Bincer, B. Durand, L. Durand, M. Ebel, C. Goebel, A. Jourjine, and P. Stevenson

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Scope of Work

The research activities of the Wisconsin theory group include a number of projects in the theory of strong interactions (new effective potential methods in field theory, theory of relativistic $q\bar{q}$ bound states, methods for the determination of α_s, investigation of the dual structure of gauge theories, development of methods to treat soft processes in quantum chromodynamics), the electroweak interactions (monopoles, weak mixing, left-right models, unified models), group theory, and particle symmetries, including problems related to the early evolution of the universe, and problems in applied mathematics relevant to particle physics. The group has made significant theoretical contributions in each of these areas.

The theory group also provides direct theoretical support for several experimental projects at Wisconsin (monopole search, studies of A dependence in strong and electroweak interactions, astrophysical questions related to the γ ray telescope project) and serves as a source of general theoretical information. It interacts with the Wisconsin phenomenology group on problems of common interest and with theorists in other areas in which similar problems or mathematical techniques arise (astrophysics, nuclear theory, statistical mechanics, and areas in mathematics).

Goals and/or Major Results to Date

Important recent results of the Wisconsin theoretical physics program include: (1) the elucidation of the structure and limitations of the QCD sum rules used to predict hadronic masses; (2) a demonstration that the coupling of the magnetic monopole "runs", contrary to arguments advanced in the past; (3) development of very efficient new methods for numerical solution of relativistic wave equations, and application to quarkonium systems; (4) complete investigations of experimental constraints on left-right mixing models for electroweak interactions; (5) systematic development of tensor operators and missing label operators for the classical Lie algebras and supersymmetry algebras used in unified theories; and (6) development of a powerful new "Gaussian effective potential" approach to quantum field theory.

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Title of Project: Phenomenology Task

Person in Charge: V. Barger

Scientific and Professional Staff: V. Barger, D. B. Cline, F. Halzen, M. G. Olsson, and D. D. Reeder

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Scope of Work

The phenomenology program in high energy physics at the University of Wisconsin covers a wide range of research activities in weak, electromagnetic, and strong interactions. The pursuit of research relevant to the interpretation of experimental data and to the design of new experiments is the primary mission of this program. The emphasis is on the formulation and verification of ideas and solutions to important research questions on the frontier of particle physics. Often this involves the systematic analysis of experimental data and the evaluation of theoretical models relevant to experimental results. Their work is centered on the implications of gauge theories and their unification, for the description of particle physics phenomena. Research activities in recent or current periods have included the following areas: heavy-quark, weak-boson, and heavy-lepton production, supersymmetry, electroweak gauge models, grand unification, quark matter and cosmic rays, astrophysics, perturbative QCD, and heavy-quark bound state physics.

Goals and/or Major Results to Date

The basic goals of their phenomenology research group are to confront gauge theories of particle interactions with experimental data and to design systematic searches for new quarks, leptons, or new interactions at present and future accelerator facilities. They have made predictions and analyses regarding the important discoveries at the CERN $p\bar{p}$ collider.

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Title of Project: Study of e^+e^- Colliding Beam Physics with the TASSO Detector at PETRA (DESY)

Person in Charge: S. L. Wu

Scientific and Professional Staff: G. Baranko, A. Caldwell, M. Cherney, J. M. Izen, M. Mermikides, S. Ritz, G. Rudolph, D. Strom, M. Takashima, H. Venkataramania, E. Wicklund, S. L. Wu, and G. Zobernig

Scope of Work

This group has been working on e^+e^- colliding beam physics at the accelerator PETRA (Positron-Electron Tandem Ring Accelerator) at DESY, Hamburg, Germany. In collaboration with physicists from England, Germany and Israel, they have constructed and operated since 1978 the detector TASSO (Two-Arm Spectrometer Solenoid). Its features are a high precision vertex detector for lifetime measurement, a large charged-particle tracking chamber for momentum measurement, a large solenoid, a lead-liquid argon calorimeter for identification and energy measurement of electrons and photons, muon chambers, and a two-arm spectrometer with Cerenkov counters for pion, kaon, and proton identification. The TASSO experiment is instrumental to the test of electroweak theory, the test of theory of quantum chromodynamics, the study of jet phenomena, the measurements of lifetimes of charm and bottom mesons and the search of new particles. At present, PETRA runs at the world's highest e^+e^- center-of-mass energy of 46 GeV. Thus, there is the exciting possibility of discovering new phenomena at PETRA in the near future.

Goals and/or Major Results to Date

The main physics goal of this experiment is the discovery of new phenomena. Some of the physics results with this group playing a prominent role are: 1) discovery of the gluon through three-jet events; this group made a major contribution to the first evidence of the three-jet events which signified the existence of gluons; 2) first determination of the spin of the gluon; 3) first measurement of the π^0 inclusive cross section; 4) observation of the unexpected copious production of baryons; 5) measurement of jet fragmentation parameters; 6) determination of the quark-gluon strong coupling constant α_S, in both first and second orders; 7) test of flavor independence of α_S; 8) observation of weak and electromagnetic interference for lepton and quark pair production; 9) search for technipions and charged Higgs through the hadronic decay modes; 10) tagging of charmed quark events through the meson $D^{*\pm}$;11) tagging of bottom quark events from inclusive electrons; 12) measurements of heavy quark fragmentation; and 13) measurements of lifetimes of charm and bottom mesons. Since 1979 the TASSO Collaboration has published about 50 papers in refereed physics journals.

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Title of Project: Ultra High Energy Gamma Rays

Person in Charge: W. Fry

Scientific and Professional Staff: U. Camerini, R. March, J. Matthews, R. Morse, D. Reeder, A. Szentgyorgyi, and A. Tsirou

Scope of Work

A collaboration has been formed comprising the Universities of Athens, Hawaii, Purdue, and Wisconsin to build an Ultra High Energy Gamma Ray facility at Haleakala, Hawaii. The telescope utilizes the Cerenkov' light from electrons in an air shower. A single gamma ray entering the earth's atmosphere can be detected by this technique if its energy is greater than 2×10^{11} e.v. The telescope facility consists of 6 mirrors, 2 ft. in diameter with 6 Hamamatsu phototubes at the focal point of each mirror. Although a few similar telescopes are in operation, none operate at the single photoelectron level and with a time resolution comparable to this facility. Because of these two fundamental innovations, the energy threshold will be considerably lower than existing facilities, making data acquisition an order of magnitude faster.

Goals and/or Major Results to Date

There are two major goals that they wish to achieve with this facility; namely:

1. A study of ultra high energy gamma rays from astrophysical sources such as pulsars, accreting stars, external galaxies and quasars. With fast timing and fast data acquisition they will be able to study some of the physical properties of these sources and their surrounding environment.

2. The Cerenkov' light techniques permit a study of high energy interaction of primary cosmic rays at the top of the atmosphere and their associated gamma ray production. Some information will be obtained on the properties of air showers.

The telescope facility, although not completely finished, is in operation on Haleakala. The equatorial mount has been tested with its computer controlled drive. The fast electronics for 9 (of the 36 total) phototubes are in operation and the coincidence circuitry has provided preliminary data acquisition on tapes. The multifold coincidence rates that were found were in excellent agreement with the predicted Monte Carlo results. Data on astrophysical sources is expected to begin in October.

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Title of Project: Electromagnetic Interactions Using the Electron Accelerator and Storage Ring at SLAC

Person in Charge: R. Prepost

Scientific and Professional Staff: M. Delfino, J. Johnson, T. Lavine, T. Maruyama, R. Prepost, and B. Heltsley

Scope of Work; Goals and/or Major Results to Date

The major part of this task is the operation of the MAC detector at the PEP storage ring. The MAC detector is one of the detectors at the PEP storage ring used for the study of high energy electron-positron collisions. This detector is operated as a collaboration between groups from the University of Wisconsin, The University of Colorado, Northeastern University, The University of Houston, Stanford University, SLAC, The University of Utah, and the Frascati National Laboratory of Italy.

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Madison, Wisconsin

The MAC detector incorporates 4 pi electromagnetic and hadron calorimetry with 4 pi muon tracking through 1 meter of magnetized steel. The inner region surrounding the beam pipe is instrumented with a 900 cell drift chamber with dE/dx capability, a small angle tagging system for new particle searches, and a recently installed vertex chamber around the 7.6 cm beam pipe.

Members of this group are also active in R&D and construction for the SLD detector to be used at the Stanford Linear Collider. Wisconsin is active in the Uranium calorimetry R&D and in design and test aspects of the Iarocci tube system for the iron calorimeter. The Wisconsin group has also been involved in planning for beam polarization and measurement and may eventually take responsibility for a polarization measurement system.

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Title of Project: Hyperon Beam Program at Fermilab

Person in Charge: L. G. Pondrom

Scientific and Professional Staff: R. Handler and M. Sheaff

Scope of Work; Goals and/or Major Results to Date

The Fermilab "neutral" hyperon beam program, which has included experiments with charged hyperons, has been an extended project, covering ten separately approved experiments in as many years at the Laboratory. The most important work has centered on the magnetic moments of the hyperons Λ, Σ^+, Σ^-, Ξ^0, and Ξ^-. The discovery of polarization in the early stages of the Λ experiments led to a new level of precision in magnetic moment measurements, which has strengthened the quark model of baryon structure. Other results include systematic studies of the polarization itself, as well as production cross sections from various target nuclei: hydrogen, beryllium, copper, and lead.

The effort in the past year has concentrated on a synthesis of a very large amount of data on these diverse phenomena. The constituent quark model baryon wave functions, gives a better than qualitative account of all of the observed effects.

The original apparatus, now 12 years old, is still in use by other members of the original collaboration in a study of K_S^0 decays. Fermilab E-621. A future project, Fermilab P-732, has been proposed to search for the forbidden decay $\Xi^0 \rightarrow p + \pi^-$ at a level of one part in 10^8.

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UNIVERSITY OF WISCONSIN
Madison, Wisconsin

Award No.: AC02-82ER40077

Title of Project: The Critical Current Density, The Fabrication Process and the Microstructure in Superconducting Composites of Nb-Ti for High Energy Physics

Person in Charge: D. C. Larbalestier

Scientific and Professional Staff: A. W. West, W. S. Starch, W. Warnes, and C. Meingast

Scope of Work

The group is studying superconducting composites of Nb-Ti with a view to understanding and improving the critical current densities of such composites. The research is being carried out both with experimental composites which are fabricated and evaluated entirely within their own laboratories, as well as with industrially fabricated material. The key feature of their work is their ability to control the fabrication process, to perform the microstructural characterization of heavily cold-worked composites, and to measure their superconducting properties.

Goals and/or Major Results to Date

A major step has been the identification of the deleterious effect of microchemical inhomogeneities present in Nb-Ti on the critical current density. Such defects produce significant non-uniformity in the cold-worked substructure of the superconductor, this then being responsible for a great spread in α-Ti precipitate size produced by optimizing heat treatments. The beneficial effects of utilizing homogeneous Nb-Ti have now been demonstrated, both in the laboratory and on an industrial scale. The homogeneous material has so far produced about 25 percent increase in J_c. They have also been able to image and characterize the microstructure of high J_c composites for the first time and it appears that they shall soon be able to formulate quantitative relationships between the J_c and the microstructure.

The overall goal is to probe the limits to J_c in Nb-Ti composites and to push as close as is practically feasible to these limits by collaboration with the industrial superconducting manufacturers.

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YALE UNIVERSITY
New Haven, Connecticut

Award No.: DE-AC02-76ER03075

Title of Project: Research in Experimental Elementary Particle Physics

Persons in Charge: R. K. Adair and J. Sandweiss

Scientific and Professional Staff: P. Cooper, R. Majka, J. Sandweiss, A. J. Slaughter, L. Teig, R. Lauer, P. Martin, O. Murphy, S. Dhawan, and A. Disco

Scope of Work; Goals and/or Major Results to Date

This group has carried on two major efforts for the last six years. The first is a major program of research and development of the high resolution streamer chamber technique for charmed and beauty particle physics. The second is a program of research using the Fermilab hyperon beam which was developed earlier by the group in collaboration with Fermilab colleagues.

The streamer chamber has been used in an experiment, recently completed, which measured charmed particle production by 300 GeV neutrons. Also, they have developed a second generation chamber which has a track measurement precision of ~5μm and a two track submitted resolution of ~30μm. A proposal for a new experiment has been submitted to FNAL. They believe this new instrument will open many new experimental opportunities for heavy quark studies at the Tevatron. The hyperon measurements include a survey of hyperon production, measurement of Σ^+, Σ^- and Ξ magnetic moments. A recently completed experiment, still in analysis, will measure the asymmetry in the leptonic decay of polarized Σ^- hyperons. This measurement is the one remaining problem with the standard Cabbibo mixing theory at the electroweak coupling of the light quarks. Previous measurements, with poor statistics, have disagreed with the theory. A definitive result will be available soon from the new experiment.

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Title of Project:

Person in Charge: M. P. Schmidt

Scientific and Professional Staff: R. K. Adair, J. K. Black, H. Kasha, M. P. Schmidt, R. Lauer, P. Martin, and O. Murphy

Scope of Work; Goals and/or Major Results to Date

For the last six years (and for the next few years) this group has been conducting experiments concerned with rare K-decays. They have been especially interested in making accurate measurements of CP-violating effects which serve to constrain and illuminate CP-violation in conventional models of the weak interactions. More recently they have been concerned with measurements of flavor changing currents which bear on GUTS theories such as possible quark substructures as suggested in systems such as the Technicolor models.

In the course of the last few years, this group has established that the CP-violating polarizatin of muons normal to the plane of decay in $K_L\to\pi+\mu+\nu$ decays, and $K^+\to\pi+\mu+\nu$ decays, is quite small demonstrating that the phase between muon helicity states is smaller than the canonical CP-violation parameter, $|\eta|-2.3\cdot 10^{-3}$. A measurement, just concluded, of the CP-violating parameter $\varepsilon'/\varepsilon=0.0017\pm0.0082$, is of considerable interest inasmuch as the results exclude certain attractive classes of models of CP-violation. At the present time, the group is preparing to measure the flavor-changing decay, $K_L^0\to\mu+e$ to an accuracy such that a branching ratio as large of 10^{-10} should be seen. Interesting sets of Technicolor type models predict that the decay should occur at that level.

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Title of Project: Rare Kaon Decay Physics

Person in Charge: M. E. Zeller

Scientific and Professional Staff: N. Hadley, W. D. Herold, L. Trudell, C. Campagnari, M. McGuigan, S. Axelrod, and R. Morrison

Scope of Work; Goals and/or Major Results to Date

This group has been performing experiments at Brookhaven National Laboratory for approximately eight years. Beginning with spin physics in kaon nucleon system and later studying the properties of sigma hyperon production and decays at low energies, they are now preparing an experiment to search for the rare decay $K^+\to\pi^+\mu^+e^-$. In their recently completed experiment they have measured the production of kaons from complex nuclei by 28 GeV protons near 700 MeV/c and 0°. These results, along with a phenomenological model describing the data are being prepared for publication. They have also measured sigma hyperon production near 700 MeV/c and 180°, and these results are also in preparation.

Their present project is to search for the rare decay $K^+\to\pi^+\mu^+e^-$ to a level of 10^{-11} in branching ratio. This experiment is being performed in collaboration with colleagues from BNL, the University of Washington, and SIN. They have designed a spectrometer system capable of examining 10^5 decays per machine pulse. With this device they will improve upon the present branching ratio limit of 5×10^{-9} in roughly two hours of machine time. Such leptonic flavor changing decays are presently of great interest in their attempts to understand the underpinnings of spontaneous symmetry breaking. Theirs is the first in a series of experiments at BNL along these lines. They will also make equivalently significant improvements on measurements of the decays $K^+\rightarrow\pi^+e^+e^-$ and $\pi^0\rightarrow e^+e^-$.

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Title of Project: Deep Inelastic Muon Scattering and High Energy Polarization Phenomena

Person in Charge: V. Hughes

Scientific and Professional Staff: V. Hughes, P. Schuler, D. Lu, R. Oppenheim, V. Harsh, C. Liu, V. Papavassiliou, R. Piegaia, S. Dhawan, and L. Trudell

Scope of Work; Goals and/or Major Results to Date

In the recent past this group has completed two major series of experiments with high energy polarized electrons at SLAC. One has involved the measurement of spin-dependent asymmetries in the deep inelastic (and resonance region) scattering of polarized electrons by polarized protons and has led to the determination of the internal spin structure of the proton. The other (with SLAC group A) involved the scattering of polarized electrons by unpolarized nucleons and led to the discovery of parity nonconservation in the electroweak interactions. Developments on polarized electron sources and polarized proton targets accompanied these experiments.

At present this group is collaborating with the EMC group at CERN to measure the spin dependence proton structure functions by deep inelastic polarized μ-p scattering. Data were observed this past summer and further data-taking is planned in 1985. The muon results will extend the kinematics over which the spin dependent structure function is known and hence provide a more sensitive tests of the Bjorken polarization sum rule, of scaling and of nucleon models. They are also working on FNAL E-665, the Tevatron deep inelastic muon scattering experiment. In particular, they are designing and constructing the large ring imaging Cerenkov counter. The FNAL E-665 detector is designed to provide a quite complete analysis of the final state hadrons and will allow a rich program in the study of deep inelastic muon scattering at the highest available laboratory energies. Their own physics interest is oriented towards the study of structure functions and polarization phenomena.

At Brookhaven recently, they have undertaken a study of the possibility of a muon g-2 measurement of the AGS to a precison level of 0.3 ppm. They have been, and are now also, engaged in some developments associated with the polarized proton beam at the AGS.

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YALE UNIVERSITY
New Haven, Connecticut

Title of Project: Theoretical Research on Elementary Particles and Interactions

Persons in Charge: T. Appelquist, F. Gursey, S. W. MacDowell, and C. M. Sommerfield

Scientific and Professional Staff: M. Bowick, A. Chodos, R. Shankar, H. C. Tze, and L.C.R. Wijewardhana

Scope of Work; Goals and/or Major Results to Date

The general context of the particle theory work at Yale is gauge field theories in their various fundamental aspects. This includes dynamics, local and global symmetry properties, grand unified theories, unification with gravity through Kaluza-Klein scenarios or through extended supergravity, and theories of Higgs and fermion substructure. There is also great current interest in soluble two-dimensional models and in correspondences between four-dimensional and two-dimensional theories. In addition, there is a great deal of interdisciplinary work on the representation theory of groups and supergroups with applications to nuclear physics, scattering problems, the transfer matrix, etc.

Some highlights of recent years include the construction of exact monopole solutions (Prasad and Sommerfield, 1975), the suggestion that grand unified theories be based on exceptional groups (Gursey and collaborators, 1976), the analysis of strongly interacting Higgs bosons (Appelquist and Bernard 1980), the establishment of the relation between the statistical mechanical free energy and the s-matrix in the corresponding two-dimensional field theories (Shankar, 1981), the first suggesion that a viable cosmological model could be developed in the context of Kaluza-Klein theories (Chodos and Detweiler, 1979) and the observation that quantum, Casimir energy effects could play an important role in compactifying the extra dimensions in Kaluza-Klein theories (Appelquist and Chodos, 1983).

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